Bayesian Methods & Multiclass

Mengye Ren

NYU

Oct 29, 2023

Announcement

- Schedule your project consultation soon (they are on the week after the proposal).
- Use the provided template! (if your final report fails to use template then there will be marks off)
- Homework 3 will be released soon and due Nov 12 11:59AM.

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters
- Bayes Rule:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$$

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters
- Bayes Rule:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$$

-

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

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters
- Bayes Rule:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$$

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

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters
- Bayes Rule:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$$

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

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

Recap

- Bayesian modeling adds a prior on the parameters.
- Models the distribution of parameters
- Bayes Rule:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$$

-

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

-

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

- Conjugate prior: Having the same form of distribution as the posterior.

Bayesian Point Estimates

- We have the posterior distribution $\theta \mid \mathcal{D}$.
- What if someone asks us to choose a single $\hat{\theta}$ (i.e. a point estimate of θ)?

Bayesian Point Estimates

- We have the posterior distribution $\theta \mid \mathcal{D}$.
- What if someone asks us to choose a single $\hat{\theta}$ (i.e. a point estimate of θ)?
- Common options:

Bayesian Point Estimates

- We have the posterior distribution $\theta \mid \mathcal{D}$.
- What if someone asks us to choose a single $\hat{\theta}$ (i.e. a point estimate of θ)?
- Common options:
  - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$

Bayesian Point Estimates

- We have the posterior distribution $\theta \mid \mathcal{D}$.
- What if someone asks us to choose a single $\hat{\theta}$ (i.e. a point estimate of θ)?
- Common options:
  - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$
  - **maximum a posteriori (MAP) estimate** $\hat{\theta} = \arg\max_\theta p(\theta \mid \mathcal{D})$
    - Note: this is the **mode** of the posterior distribution

What else can we do with a posterior?

- Look at it: display uncertainty estimates to our client

What else can we do with a posterior?

- Look at it: display uncertainty estimates to our client
- Extract a **credible set** for θ (a Bayesian confidence interval).
  - e.g. Interval $[a, b]$ is a 95% **credible set** if

$$\mathbb{P}(\theta \in [a, b] \mid \mathcal{D}) \geqslant 0.95$$

What else can we do with a posterior?

- Look at it: display uncertainty estimates to our client
- Extract a **credible set** for θ (a Bayesian confidence interval).
  - e.g. Interval $[a, b]$ is a 95% **credible set** if

$$\mathbb{P}(\theta \in [a, b] \mid \mathcal{D}) \geqslant 0.95$$

- Select a point estimate using **Bayesian decision theory**:
  - Choose a loss function.
  - Find action **minimizing expected risk w.r.t. posterior**

Bayesian Decision Theory

Bayesian Decision Theory

- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$.
  - **Loss function**: $\ell : \mathcal{A} \times \Theta \to \mathrm{R}$.

Bayesian Decision Theory

- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$.
  - **Loss function**: $\ell : \mathcal{A} \times \Theta \to \mathrm{R}$.
- The **posterior risk** of an action $a \in \mathcal{A}$ is

$$r(a) \quad := \quad \mathbb{E}\left[\ell(\theta, a) \mid \mathcal{D}\right]$$

Bayesian Decision Theory

- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$.
  - **Loss function**: $\ell : \mathcal{A} \times \Theta \to R$.
- The **posterior risk** of an action $a \in \mathcal{A}$ is

$$
\begin{aligned}
r(a) &:= \mathbb{E}\left[\ell(\theta, a) \mid \mathcal{D}\right] \\
&= \int \ell(\theta, a) p(\theta \mid \mathcal{D})\, d\theta.
\end{aligned}
$$

Bayesian Decision Theory

- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$.
  - **Loss function**: $\ell : \mathcal{A} \times \Theta \to \mathbf{R}$.
- The **posterior risk** of an action $a \in \mathcal{A}$ is

$$
\begin{aligned}
r(a) &:= \mathbb{E}\left[\ell(\theta, a) \mid \mathcal{D}\right] \\
&= \int \ell(\theta, a) p(\theta \mid \mathcal{D})\, d\theta.
\end{aligned}
$$

  - It's the **expected loss under the posterior.**

Bayesian Decision Theory

- Ingredients:
  - **Parameter space** Θ.
  - **Prior**: Distribution $p(\theta)$ on Θ.
  - **Action space** $\mathcal{A}$.
  - **Loss function**: $\ell : \mathcal{A} \times \Theta \to \mathrm{R}$.
- The **posterior risk** of an action $a \in \mathcal{A}$ is

$$\begin{aligned} r(a) &:= \mathbb{E}\left[\ell(\theta, a) \mid \mathcal{D}\right] \\ &= \int \ell(\theta, a) p(\theta \mid \mathcal{D})\, d\theta. \end{aligned}$$

  - It's the **expected loss under the posterior.**
- A **Bayes action** a^* is an action that minimizes posterior risk:

$$r(a^*) = \min_{a \in \mathcal{A}} r(a)$$

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
  - We want to produce a **point estimate** for θ.

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
  - We want to produce a **point estimate** for θ.
- Choose:

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
  - We want to produce a **point estimate** for θ.
- Choose:
  - **Prior** $p(\theta)$ on $\Theta = \mathrm{R}$.

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
  - We want to produce a **point estimate** for θ.
- Choose:
  - **Prior** $p(\theta)$ on $\Theta = \mathbf{R}$.
  - **Loss** $\ell(\hat{\theta}, \theta)$

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
  - We want to produce a **point estimate** for θ.
- Choose:
  - **Prior** $p(\theta)$ on $\Theta = \mathrm{R}$.
  - **Loss** $\ell(\hat{\theta}, \theta)$
- Find **action** $\hat{\theta} \in \Theta$ that minimizes the **posterior risk:**

$$r(\hat{\theta}) = \mathbb{E}\left[\ell(\hat{\theta}, \theta) \mid \mathcal{D}\right]$$

Bayesian Point Estimation

- General Setup:
  - Data $\mathcal{D}$ generated by $p(y \mid \theta)$, for unknown $\theta \in \Theta$.
  - We want to produce a **point estimate** for θ.
- Choose:
  - **Prior** $p(\theta)$ on $\Theta = \mathrm{R}$.
  - **Loss** $\ell(\hat{\theta}, \theta)$
- Find **action** $\hat{\theta} \in \Theta$ that minimizes the **posterior risk:**

$$
\begin{aligned}
r(\hat{\theta}) &= \mathbb{E}\left[\ell(\hat{\theta}, \theta) \mid \mathcal{D}\right] \\
&= \int \ell(\hat{\theta}, \theta) p(\theta \mid \mathcal{D})\, d\theta
\end{aligned}
$$

Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ posterior mode
- Absolute Loss : $\ell(\hat{\theta}, \theta) = \left|\theta - \hat{\theta}\right| \quad \Rightarrow$ posterior median

Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ posterior mode
- Absolute Loss : $\ell(\hat{\theta}, \theta) = \left|\theta - \hat{\theta}\right| \quad \Rightarrow$ posterior median
- Optimal decision depends on the loss function and the posterior distribution.

Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ posterior mode
- Absolute Loss : $\ell(\hat{\theta}, \theta) = \left|\theta - \hat{\theta}\right| \quad \Rightarrow$ posterior median
- Optimal decision depends on the loss function and the posterior distribution.
- Example: I have a card drawing from a deck of 2,3,3,4,4,5,5,5, and you guess the value of my card.

Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ posterior mode
- Absolute Loss : $\ell(\hat{\theta}, \theta) = \left|\theta - \hat{\theta}\right| \quad \Rightarrow$ posterior median
- Optimal decision depends on the loss function and the posterior distribution.
- Example: I have a card drawing from a deck of 2,3,3,4,4,5,5,5, and you guess the value of my card.
- mean: 3.875; mode: 5; median: 4

Bayesian Point Estimation: Square Loss

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

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

Bayesian Point Estimation: Square Loss

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

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

- Differentiate:

$$\frac{dr(\hat{\theta})}{d\hat{\theta}} = -\int 2\left(\theta - \hat{\theta}\right) p(\theta \mid \mathcal{D})\, d\theta$$

Bayesian Point Estimation: Square Loss

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

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

- Differentiate:

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

Bayesian Point Estimation: Square Loss

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

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

- Differentiate:

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

Bayesian Point Estimation: Square Loss

- Derivative of posterior risk is

$$\frac{dr(\hat{\theta})}{d\hat{\theta}} = -2\int \theta p(\theta \mid \mathcal{D})\, d\theta + 2\hat{\theta}.$$

Bayesian Point Estimation: Square Loss

- Derivative of posterior risk is

$$\frac{dr(\hat{\theta})}{d\hat{\theta}} = -2\int \theta p(\theta \mid \mathcal{D})\, d\theta + 2\hat{\theta}.$$

- First order condition $\frac{dr(\hat{\theta})}{d\hat{\theta}} = 0$ gives

$$\hat{\theta} \quad = \quad \int \theta p(\theta \mid \mathcal{D})\, d\theta$$

Bayesian Point Estimation: Square Loss

- Derivative of posterior risk is

$$\frac{dr(\hat{\theta})}{d\hat{\theta}} = -2\int \theta p(\theta \mid \mathcal{D})\, d\theta + 2\hat{\theta}.$$

- First order condition $\frac{dr(\hat{\theta})}{d\hat{\theta}} = 0$ gives

$$\begin{aligned} \hat{\theta} &= \int \theta p(\theta \mid \mathcal{D})\, d\theta \\ &= \mathbb{E}[\theta \mid \mathcal{D}] \end{aligned}$$

Bayesian Point Estimation: Square Loss

- Derivative of posterior risk is

$$\frac{dr(\hat{\theta})}{d\hat{\theta}} = -2\int \theta p(\theta \mid \mathcal{D})\, d\theta + 2\hat{\theta}.$$

- First order condition $\frac{dr(\hat{\theta})}{d\hat{\theta}} = 0$ gives

$$\begin{aligned} \hat{\theta} &= \int \theta p(\theta \mid \mathcal{D})\, d\theta \\ &= \mathbb{E}[\theta \mid \mathcal{D}] \end{aligned}$$

- The **Bayes action** for **square loss** is the posterior mean.

Interim summary

Recap and Interpretation

- The prior represents belief about θ before observing data $\mathcal{D}$.
- The posterior represents **rationally updated beliefs** after seeing $\mathcal{D}$.

Recap and Interpretation

- The prior represents belief about θ before observing data $\mathcal{D}$.
- The posterior represents **rationally updated beliefs** after seeing $\mathcal{D}$.
- All inferences and action-taking are based on the posterior distribution.

Recap and Interpretation

- The prior represents belief about θ before observing data $\mathcal{D}$.
- The posterior represents **rationally updated beliefs** after seeing $\mathcal{D}$.
- All inferences and action-taking are based on the posterior distribution.
- In the Bayesian approach,
  - No issue of justifying an estimator.

Recap and Interpretation

- The prior represents belief about θ before observing data $\mathcal{D}$.
- The posterior represents **rationally updated beliefs** after seeing $\mathcal{D}$.
- All inferences and action-taking are based on the posterior distribution.
- In the Bayesian approach,
    - No issue of justifying an estimator.
    - Only choices are
        - **family of distributions**, indexed by Θ, and
        - **prior distribution** on Θ

Recap and Interpretation

- The prior represents belief about θ before observing data $\mathcal{D}$.
- The posterior represents **rationally updated beliefs** after seeing $\mathcal{D}$.
- All inferences and action-taking are based on the posterior distribution.
- In the Bayesian approach,
  - No issue of justifying an estimator.
  - Only choices are
    - **family of distributions**, indexed by Θ, and
    - **prior distribution** on Θ
  - For decision making, we need a **loss function**.

Recap: Conditional Probability Models

Conditional Probability Modeling

- **Input space** $\mathcal{X}$
- **Outcome space** $\mathcal{Y}$
- **Action space** $\mathcal{A} = \{p(y) \mid p \text{ is a probability distribution on } \mathcal{Y}\}$.

Conditional Probability Modeling

- **Input space** $\mathcal{X}$
- **Outcome space** $\mathcal{Y}$
- **Action space** $\mathcal{A} = \{p(y) \mid p \text{ is a probability distribution on } \mathcal{Y}\}$.
- **Hypothesis space** $\mathcal{F}$ contains prediction functions $f : \mathcal{X} \to \mathcal{A}$.
- **Prediction function** $f \in \mathcal{F}$ takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$

Conditional Probability Modeling

- **Input space** $\mathcal{X}$
- **Outcome space** $\mathcal{Y}$
- **Action space** $\mathcal{A} = \{p(y) \mid p$ is a probability distribution on $\mathcal{Y}\}$.
- **Hypothesis space** $\mathcal{F}$ contains prediction functions $f : \mathcal{X} \to \mathcal{A}$.
- **Prediction function** $f \in \mathcal{F}$ takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$
- A **parametric family of conditional densities** is a set

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

  - where $p(y \mid x, \theta)$ is a density on **outcome space** $\mathcal{Y}$ for each x in **input space** $\mathcal{X}$, and
  - θ is a **parameter** in a [finite dimensional] **parameter space** Θ.

Conditional Probability Modeling

- **Input space** $\mathcal{X}$
- **Outcome space** $\mathcal{Y}$
- **Action space** $\mathcal{A} = \{p(y) \mid p \text{ is a probability distribution on } \mathcal{Y}\}$.
- **Hypothesis space** $\mathcal{F}$ contains prediction functions $f : \mathcal{X} \to \mathcal{A}$.
- **Prediction function** $f \in \mathcal{F}$ takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$
- A **parametric family of conditional densities** is a set

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

  - where $p(y \mid x, \theta)$ is a density on **outcome space** $\mathcal{Y}$ for each x in **input space** $\mathcal{X}$, and
  - θ is a **parameter** in a [finite dimensional] **parameter space** Θ.

- This is the common starting point for either classical or Bayesian regression.

- **Data:** $\mathcal{D} = (y_1, \ldots, y_n)$
- The probability density for our data $\mathcal{D}$ is

$$p(\mathcal{D} \mid x_1, \ldots, x_n, \theta) \quad = \quad \prod_{i=1}^{n} p(y_i \mid x_i, \theta).$$

Classical treatment: Likelihood Function

- **Data:** $\mathcal{D} = (y_1, \ldots, , y_n)$
- The probability density for our data $\mathcal{D}$ is

$$p(\mathcal{D} \mid x_1, \ldots, x_n, \theta) \quad = \quad \prod_{i=1}^{n} p(y_i \mid x_i, \theta).$$

- For fixed $\mathcal{D}$, the function $\theta \mapsto p(\mathcal{D} \mid x, \theta)$ is the **likelihood function**:

$$L_{\mathcal{D}}(\theta) = p(\mathcal{D} \mid x, \theta),$$

where $x = (x_1, \ldots, x_n)$.

Maximum Likelihood Estimator

- The **maximum likelihood estimator (MLE)** for θ in the family $\{p(y \mid x, \theta) \mid \theta \in \Theta\}$ is

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

- MLE corresponds to ERM, if we set the loss to be the negative log-likelihood.

Maximum Likelihood Estimator

- The **maximum likelihood estimator (MLE)** for θ in the family $\{p(y \mid x, \theta) \mid \theta \in \Theta\}$ is

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

- MLE corresponds to ERM, if we set the loss to be the negative log-likelihood.
- The corresponding prediction function is

$$\hat{f}(x) = p(y \mid x, \hat{\theta}_{\text{MLE}}).$$

Bayesian Conditional Probability Models

Bayesian Conditional Models

- Input space $\mathcal{X} = \mathbf{R}^d$ Outcome space $\mathcal{Y} = \mathbf{R}$

Bayesian Conditional Models

- Input space $\mathcal{X} = \mathbf{R}^d$ Outcome space $\mathcal{Y} = \mathbf{R}$
- The Bayesian conditional model has two components:
  - A **parametric family of conditional densities**:

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

Bayesian Conditional Models

- Input space $\mathcal{X} = \mathbf{R}^d$ Outcome space $\mathcal{Y} = \mathbf{R}$
- The Bayesian conditional model has two components:
  - A **parametric family of conditional densities**:

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

  - A **prior distribution** $p(\theta)$ on $\theta \in \Theta$.

The Posterior Distribution

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

The Posterior Distribution

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

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

The Posterior Distribution

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

$$p(\theta \mid \mathcal{D}, x) \quad \propto \quad p(\mathcal{D} \mid \theta, x) p(\theta)$$

The Posterior Distribution

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

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

The Posterior Distribution

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

The Posterior Distribution

- The **prior distribution** $p(\theta)$ represents our beliefs about θ before seeing $\mathcal{D}$.
- The **posterior distribution** for θ 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 **rationally updated beliefs** after seeing $\mathcal{D}$.
- Each θ corresponds to a prediction function,
    - i.e. the conditional distribution function $p(y \mid x, \theta)$.

Point Estimates of Parameter

- What if we want point estimates of θ?

Point Estimates of Parameter

- What if we want point estimates of θ?
- We can use **Bayesian decision theory** to derive point estimates.

Point Estimates of Parameter

- What if we want point estimates of θ?
- We can use **Bayesian decision theory** to derive point estimates.
- We may want to use
  - $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}, x]$ (the posterior mean estimate)
  - $\hat{\theta} = \text{median}[\theta \mid \mathcal{D}, x]$
  - $\hat{\theta} = \arg\max_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

Back to the basic question - Bayesian Prediction Function

- Find a function takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$

Back to the basic question - Bayesian Prediction Function

- Find a function takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$
- In the frequentist approach:
  - Choose family of conditional probability densities (hypothesis space).
  - Select one conditional probability from family, e.g. using MLE.

Back to the basic question - Bayesian Prediction Function

- Find a function takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$
- In the frequentist approach:
  - Choose family of conditional probability densities (hypothesis space).
  - Select one conditional probability from family, e.g. using MLE.
- In the Bayesian setting:

Back to the basic question - Bayesian Prediction Function

- Find a function takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$
- In the frequentist approach:
  - Choose family of conditional probability densities (hypothesis space).
  - Select one conditional probability from family, e.g. using MLE.
- In the Bayesian setting:
  - We choose a parametric family of conditional densities

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

  - and a prior distribution $p(\theta)$ on this set.

Back to the basic question - Bayesian Prediction Function

- Find a function takes input $x \in \mathcal{X}$ and produces a **distribution** on $\mathcal{Y}$
- In the frequentist approach:
  - Choose family of conditional probability densities (hypothesis space).
  - Select one conditional probability from family, e.g. using MLE.
- In the Bayesian setting:
  - We choose 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, how do we predict a distribution on y for input x?
- We don't need to make a discrete selection from the hypothesis space: we **maintain uncertainty**.

The Prior Predictive Distribution

- Suppose we have not yet observed any data.

The Prior Predictive Distribution

- Suppose we have not yet observed any data.
- In the Bayesian setting, we can still produce a prediction function.

The Prior Predictive Distribution

- Suppose we have not yet observed any data.
- In the Bayesian setting, we can still produce a prediction function.
- The **prior predictive distribution** is given by

$$x \mapsto p(y \mid x)$$

The Prior Predictive Distribution

- Suppose we have not yet observed any data.
- In the Bayesian setting, we can still produce a prediction function.
- The **prior predictive distribution** is given by

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

The Prior Predictive Distribution

- Suppose we have not yet observed any data.
- In the Bayesian setting, we can still produce a prediction function.
- The **prior predictive distribution** is given by

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

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

The Posterior Predictive Distribution

- Suppose we've already seen data $\mathcal{D}$.

The Posterior Predictive Distribution

- Suppose we've already seen data $\mathcal{D}$.
- The **posterior predictive distribution** is given by

$$x \mapsto p(y \mid x, \mathcal{D})$$

The Posterior Predictive Distribution

- Suppose we've already seen data $\mathcal{D}$.
- The **posterior predictive distribution** is given by

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

The Posterior Predictive Distribution

- Suppose we've already seen data $\mathcal{D}$.
- The **posterior predictive distribution** is given by

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

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

Comparison to Frequentist Approach

- In Bayesian statistics we have two distributions on Θ:
  - the prior distribution $p(\theta)$
  - the posterior distribution $p(\theta \mid \mathcal{D})$.

Comparison to Frequentist Approach

- In Bayesian statistics we have two distributions on Θ:
  - the prior distribution $p(\theta)$
  - the posterior distribution $p(\theta \mid \mathcal{D})$.
- These distributions over parameters correspond to distributions on the hypothesis space:

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

Comparison to Frequentist Approach

- In Bayesian statistics we have two distributions on Θ:
  - the prior distribution $p(\theta)$
  - the posterior distribution $p(\theta \mid \mathcal{D})$.
- These distributions over parameters correspond to distributions on the hypothesis space:

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

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

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

Comparison to Frequentist Approach

- In Bayesian statistics we have two distributions on Θ:
  - the prior distribution $p(\theta)$
  - the posterior distribution $p(\theta \mid \mathcal{D})$.
- These distributions over parameters correspond to distributions on the hypothesis space:

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

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

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

- In the Bayesian approach, we integrate out over Θ w.r.t. $p(\theta \mid \mathcal{D})$ and predict with

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

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.

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.
- $x \mapsto \mathbb{E}[y \mid x, \mathcal{D}]$, to minimize expected square error.

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.
- $x \mapsto \mathbb{E}[y \mid x, \mathcal{D}]$, to minimize expected square error.
- $x \mapsto \text{median}[y \mid x, \mathcal{D}]$, to minimize expected absolute error

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.
- $x \mapsto \mathbb{E}[y \mid x, \mathcal{D}]$, 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

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.
- $x \mapsto \mathbb{E}[y \mid x, \mathcal{D}]$, 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 $p(y \mid x, \mathcal{D})$.

Gaussian Regression Example

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

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?

Example in 1-Dimension: Setup

- Input space $\mathcal{X} = [-1, 1]$ Output space $\mathcal{Y} = \mathrm{R}$
- 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? R^2.

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

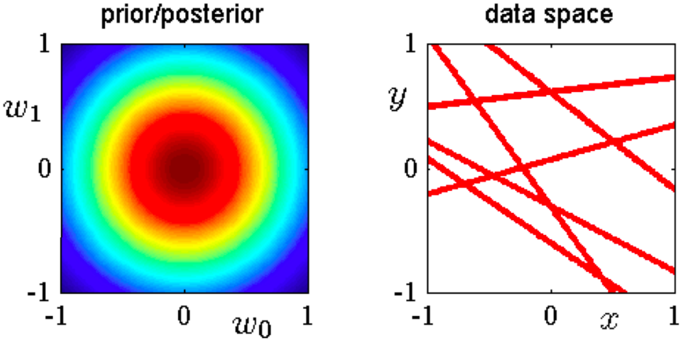
- Written another way, the **conditional probability model** is

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

- 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

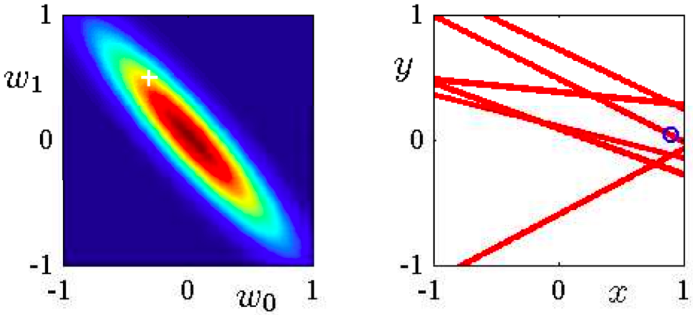
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$ (Illustrated on left)



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

Bishop's PRML Fig 3.7

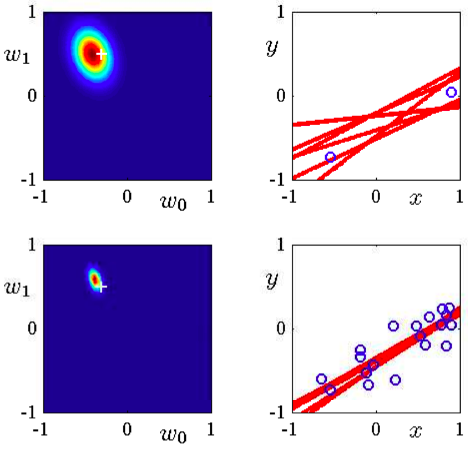
Example in 1-Dimension: 1 Observation



- On left: posterior distribution; white cross indicates true parameters
- On right:
  - blue circle indicates the training observation
  - red lines, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w|\mathcal{D})$ (posterior)

Bishop's PRML Fig 3.7

Example in 1-Dimension: 2 and 20 Observations



Bishop's PRML Fig 3.7

Gaussian Regression: Closed form

Closed Form for Posterior

- Model:

$$w \sim \mathcal{N}(0, \Sigma_0)$$

Closed Form for Posterior

- Model:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w &\ \text{i.i.d.}\ \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

Closed Form for Posterior

- Model:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w &\ \text{i.i.d.}\ \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

- Design matrix X Response column vector y

Closed Form for Posterior

- Model:

$$
\begin{aligned}
w &\sim \mathcal{N}(0, \Sigma_0) \\
y_i \mid x, w &\ \text{i.i.d.}\ \mathcal{N}(w^T x_i, \sigma^2)
\end{aligned}
$$

- Design matrix X Response column vector y
- **Posterior distribution is a Gaussian distribution:**

$$
w \mid \mathcal{D} \sim
$$

Closed Form for Posterior

- Model:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w &\text{ i.i.d. } \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

- Design matrix X Response column vector y
- **Posterior distribution is a Gaussian distribution:**

$$\begin{aligned} w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\ \mu_{\mathbf{P}} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\ \Sigma_{\mathbf{P}} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1} \end{aligned}$$

Closed Form for Posterior

- Model:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w &\text{ i.i.d. } \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

- Design matrix X Response column vector y
- **Posterior distribution is a Gaussian distribution:**

$$\begin{aligned} w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\ \mu_{\mathbf{P}} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\ \Sigma_{\mathbf{P}} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1} \end{aligned}$$

- **Posterior Variance** Σ_P gives us a natural **uncertainty measure.**

Closed Form for Posterior

- **Posterior distribution is a Gaussian distribution:**

$$w \mid \mathcal{D} \quad \sim$$

Closed Form for Posterior

- **Posterior distribution is a Gaussian distribution:**

$$
\begin{aligned}
w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\
\mu_{\mathbf{P}} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\
\Sigma_{\mathbf{P}} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1}
\end{aligned}
$$

Closed Form for Posterior

- **Posterior distribution is a Gaussian distribution:**

$$\begin{aligned} w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\ \mu_{\mathbf{P}} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\ \Sigma_{\mathbf{P}} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1} \end{aligned}$$

- If we want point estimates of w, **MAP estimator** and the **posterior mean** are given by

Closed Form for Posterior

- **Posterior distribution is a Gaussian distribution:**

$$
\begin{aligned}
w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\
\mu_{\mathbf{P}} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\
\Sigma_{\mathbf{P}} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1}
\end{aligned}
$$

- If we want point estimates of w, **MAP estimator** and the **posterior mean** are given by

$$
\hat{w} = \mu_P = \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y
$$

Closed Form for Posterior

- **Posterior distribution is a Gaussian distribution:**

$$
\begin{aligned}
w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\
\mu_{\mathbf{P}} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\
\Sigma_{\mathbf{P}} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1}
\end{aligned}
$$

- If we want point estimates of w, **MAP estimator** and the **posterior mean** are given by

$$
\hat{w} = \mu_P = \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y
$$

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

$$
\hat{w} = \mu_P = \left(X^T X + \lambda I\right)^{-1} X^T y,
$$

Closed Form for Posterior

- **Posterior distribution is a Gaussian distribution:**

$$
\begin{aligned}
w \mid \mathcal{D} &\sim \mathcal{N}(\mu_P, \Sigma_P) \\
\mu_\mathbf{P} &= \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y \\
\Sigma_\mathbf{P} &= \left(\sigma^{-2} X^T X + \Sigma_0^{-1}\right)^{-1}
\end{aligned}
$$

- If we want point estimates of w, **MAP estimator** and the **posterior mean** are given by

$$
\hat{w} = \mu_P = \left(X^T X + \sigma^2 \Sigma_0^{-1}\right)^{-1} X^T y
$$

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

$$
\hat{w} = \mu_P = \left(X^T X + \lambda I\right)^{-1} X^T y,
$$

which is of course the ridge regression solution.

Connection the MAP to Ridge Regression

- The **Posterior density** on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w \mid \mathcal{D}) \quad \propto \quad \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2}\|w\|^2\right)}_{\textbf{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\textbf{likelihood}}$$

Connection the MAP to Ridge Regression

- The **Posterior density** on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w \mid \mathcal{D}) \quad \propto \quad \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2}\|w\|^2\right)}_{\textbf{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\textbf{likelihood}}$$

- To find the **MAP**, we minimize the negative log posterior:

$$\hat{w}_{\text{MAP}} \quad = \quad \underset{w \in \mathbf{R}^d}{\arg\min}\left[-\log p(w \mid \mathcal{D})\right]$$

Connection the MAP to Ridge Regression

- The **Posterior density** on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w \mid \mathcal{D}) \quad \propto \quad \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2}\|w\|^2\right)}_{\textbf{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\textbf{likelihood}}$$

- To find the **MAP**, we minimize the negative log posterior:

$$\begin{aligned} \hat{w}_{\text{MAP}} &= \underset{w \in \mathbf{R}^d}{\arg\min} \left[-\log p(w \mid \mathcal{D})\right] \\ &= \underset{w \in \mathbf{R}^d}{\arg\min} \underbrace{\sum_{i=1}^{n} (y_i - w^T x_i)^2}_{\text{log-likelihood}} + \underbrace{\lambda \|w\|^2}_{\text{log-prior}} \end{aligned}$$

Connection the MAP to Ridge Regression

- The **Posterior density** on w for $\Sigma_0 = \frac{\sigma^2}{\lambda} I$:

$$p(w \mid \mathcal{D}) \quad \propto \quad \underbrace{\exp\left(-\frac{\lambda}{2\sigma^2}\|w\|^2\right)}_{\textbf{prior}} \underbrace{\prod_{i=1}^{n} \exp\left(-\frac{(y_i - w^T x_i)^2}{2\sigma^2}\right)}_{\textbf{likelihood}}$$

- To find the **MAP**, we minimize the negative log posterior:

$$\begin{aligned} \hat{w}_{\text{MAP}} &= \underset{w \in \mathbf{R}^d}{\arg\min}\left[-\log p(w \mid \mathcal{D})\right] \\ &= \underset{w \in \mathbf{R}^d}{\arg\min} \underbrace{\sum_{i=1}^{n}(y_i - w^T x_i)^2}_{\text{log-likelihood}} + \underbrace{\lambda\|w\|^2}_{\text{log-prior}} \end{aligned}$$

- Which is the ridge regression objective.

Predictive Posterior Distribution

- Given a new input point x_{new}, how do we predict y_{new} ?

Predictive Posterior Distribution

- Given a new input point x_{new}, how do we predict y_{new} ?
- **Predictive distribution**

$$p(y_{\textbf{new}} \mid x_{\textbf{new}}, \mathcal{D}) \quad =$$

Predictive Posterior Distribution

- Given a new input point x_{new}, how do we predict y_{new} ?
- **Predictive distribution**

$$p(y_{\mathbf{new}} \mid x_{\mathbf{new}}, \mathcal{D}) = \int p(y_{\mathbf{new}} \mid x_{\mathbf{new}}, w, \mathcal{D}) p(w \mid \mathcal{D}) \, dw$$

Predictive Posterior Distribution

- Given a new input point x_{new}, how do we predict y_{new} ?
- **Predictive distribution**

$$
\begin{aligned}
p(y_{\mathbf{new}} \mid x_{\mathbf{new}}, \mathcal{D}) &= \int p(y_{\mathbf{new}} \mid x_{\mathbf{new}}, w, \mathcal{D}) p(w \mid \mathcal{D})\, dw \\
&= \int p(y_{\mathbf{new}} \mid x_{\mathbf{new}}, w) p(w \mid \mathcal{D})\, dw
\end{aligned}
$$

Predictive Posterior Distribution

- Given a new input point x_{new}, how do we predict y_{new} ?
- **Predictive distribution**

$$
\begin{aligned}
p(y_{\textbf{new}} \mid x_{\textbf{new}}, \mathcal{D}) &= \int p(y_{\textbf{new}} \mid x_{\textbf{new}}, w, \mathcal{D}) p(w \mid \mathcal{D})\, dw \\
&= \int p(y_{\textbf{new}} \mid x_{\textbf{new}}, w) p(w \mid \mathcal{D})\, dw
\end{aligned}
$$

- For Gaussian regression, predictive distribution has closed form.

Closed Form for Predictive Distribution

- **Model**:

$$w \sim \mathcal{N}(0, \Sigma_0)$$

Closed Form for Predictive Distribution

- **Model**:

$$\begin{array}{rcl} w & \sim & \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w & \text{i.i.d.} & \mathcal{N}(w^T x_i, \sigma^2) \end{array}$$

Closed Form for Predictive Distribution

- **Model**:

$$
\begin{aligned}
w &\sim \mathcal{N}(0, \Sigma_0) \\
y_i \mid x, w &\ \text{i.i.d.}\ \mathcal{N}(w^T x_i, \sigma^2)
\end{aligned}
$$

- **Predictive Distribution**

$$
p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} \mid x_{\text{new}}, w) p(w \mid \mathcal{D})\, dw.
$$

  - Averages over prediction for each w, weighted by posterior distribution.

Closed Form for Predictive Distribution

- **Model**:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w &\quad \text{i.i.d.} \quad \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

- **Predictive Distribution**

$$p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} \mid x_{\text{new}}, w) p(w \mid \mathcal{D})\, dw.$$

  - Averages over prediction for each w, weighted by posterior distribution.

- **Closed form:**

$$y_{\text{new}} \mid x_{\text{new}}, \mathcal{D} \sim \mathcal{N}\left(\eta_{\text{new}}, \sigma^2_{\text{new}}\right)$$

Closed Form for Predictive Distribution

- **Model**:

$$\begin{aligned} w &\sim \mathcal{N}(0, \Sigma_0) \\ y_i \mid x, w \quad &\text{i.i.d.} \quad \mathcal{N}(w^T x_i, \sigma^2) \end{aligned}$$

- **Predictive Distribution**

$$p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} \mid x_{\text{new}}, w) p(w \mid \mathcal{D})\, dw.$$

  - Averages over prediction for each w, weighted by posterior distribution.

- **Closed form:**

$$\begin{aligned} y_{\text{new}} \mid x_{\text{new}}, \mathcal{D} &\sim \mathcal{N}\left(\eta_{\text{new}}, \sigma^2_{\text{new}}\right) \\ \eta_{\text{new}} &= \mu_P^T x_{\text{new}} \end{aligned}$$

Closed Form for Predictive Distribution

- **Model**:

$$
\begin{aligned}
w &\sim \mathcal{N}(0, \Sigma_0) \\
y_i \mid x, w &\quad \text{i.i.d.} \quad \mathcal{N}(w^T x_i, \sigma^2)
\end{aligned}
$$

- **Predictive Distribution**

$$
p(y_{\text{new}} \mid x_{\text{new}}, \mathcal{D}) = \int p(y_{\text{new}} \mid x_{\text{new}}, w) p(w \mid \mathcal{D})\, dw.
$$

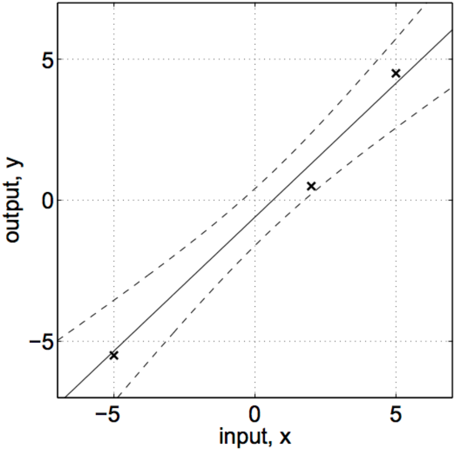
  - Averages over prediction for each w, weighted by posterior distribution.

- **Closed form:**

$$
\begin{aligned}
y_{\text{new}} \mid x_{\text{new}}, \mathcal{D} &\sim \mathcal{N}\left(\eta_{\text{new}}\,,\, \sigma^2_{\text{new}}\right) \\
\eta_{\text{new}} &= \mu_P^T x_{\text{new}} \\
\sigma^2_{\text{new}} &= \underbrace{x_{\text{new}}^T \Sigma_P x_{\text{new}}}_{\text{from variance in } w} + \underbrace{\sigma^2}_{\text{inherent variance in } y}
\end{aligned}
$$

Bayesian Regression Provides Uncertainty Estimates

- With predictive distributions, we can give mean prediction with error bands:



Rasmussen and Williams' *Gaussian Processes for Machine Learning*, Fig.2.1(b)

Multi-class Overview

Motivation

- So far, most algorithms we've learned are designed for binary classification.

Motivation

- So far, most algorithms we've learned are designed for binary classification.
- Many real-world problems have more than two classes.

Motivation

- So far, most algorithms we've learned are designed for binary classification.
- Many real-world problems have more than two classes.
- What are some potential issues when we have a large number of classes?

Today's lecture

- How to *reduce* multiclass classification to binary classification?
  - We can think of binary classifier or linear regression as a black box. Naive ways:
  - E.g. multiple binary classifiers produce a binary code for each class (000, 001, 010)
  - E.g. a linear regression produces a numerical value for each class (1.0, 2.0, 3.0)

Today's lecture

- How to *reduce* multiclass classification to binary classification?
  - We can think of binary classifier or linear regression as a black box. Naive ways:
  - E.g. multiple binary classifiers produce a binary code for each class (000, 001, 010)
  - E.g. a linear regression produces a numerical value for each class (1.0, 2.0, 3.0)
- How do we *generalize* binary classification algorithm to the multiclass setting?
  - We also need to think about the loss function.

Today's lecture

- How to *reduce* multiclass classification to binary classification?
  - We can think of binary classifier or linear regression as a black box. Naive ways:
  - E.g. multiple binary classifiers produce a binary code for each class (000, 001, 010)
  - E.g. a linear regression produces a numerical value for each class (1.0, 2.0, 3.0)
- How do we *generalize* binary classification algorithm to the multiclass setting?
  - We also need to think about the loss function.
- Example of very large output space: structured prediction.
  - Multi-class: Mutually exclusive class structure.
  - Text: Temporal relational structure.

Reduction to Binary Classification

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train k binary classifiers, one for each class: $h_1, \ldots, h_k : \mathcal{X} \to \mathrm{R}$.
- Classifier h_i distinguishes class i (+1) from the rest (-1).

One-vs-All / One-vs-Rest

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train k binary classifiers, one for each class: $h_1, \ldots, h_k : \mathcal{X} \to \mathrm{R}$.
- Classifier h_i distinguishes class i (+1) from the rest (-1).

Prediction

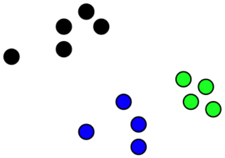
- Majority vote:

$$h(x) = \operatorname*{arg\,max}_{i \in \{1,\ldots,k\}} h_i(x)$$

- Ties can be broken arbitrarily.

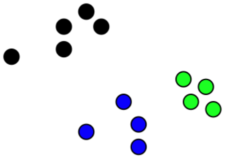
OvA: 3-class example (linear classifier)

Consider a dataset with three classes:

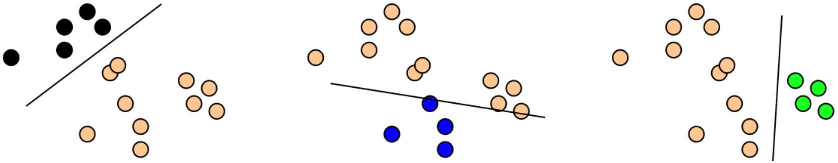


OvA: 3-class example (linear classifier)

Consider a dataset with three classes:

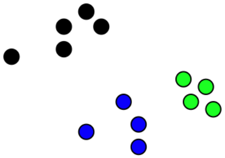


Train OvA classifiers:



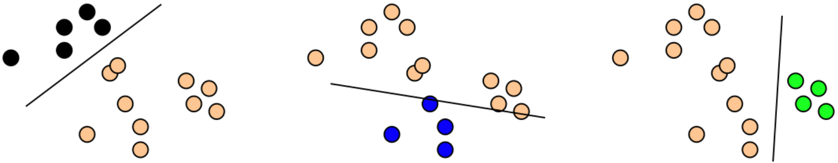
OvA: 3-class example (linear classifier)

Consider a dataset with three classes:



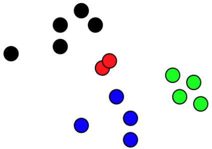
Assumption: each class is linearly separable from the rest.
Ideal case: only target class has positive score.

Train OvA classifiers:

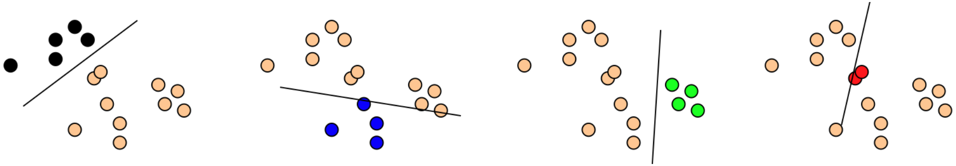


OvA: 4-class non linearly separable example

Consider a dataset with four classes:

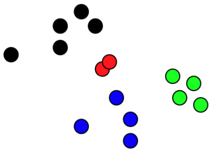


Train OvA classifiers:



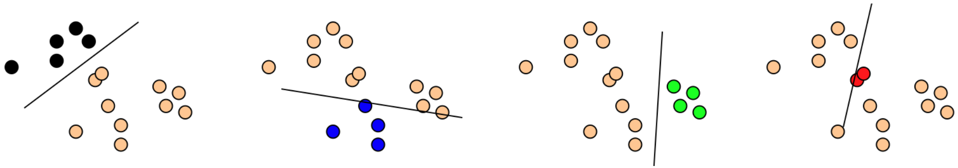
OvA: 4-class non linearly separable example

Consider a dataset with four classes:



Cannot separate red points from the rest.
Which classes might have low accuracy?

Train OvA classifiers:



All vs All / One vs One / All pairs

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

All vs All / One vs One / All pairs

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathrm{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
- Classifier h_{ij} distinguishes class i (+1) from class j (-1).

All vs All / One vs One / All pairs

Setting

- Input space: $\mathcal{X}$
- Output space: $\mathcal{Y} = \{1, \ldots, k\}$

Training

- Train $\binom{k}{2}$ binary classifiers, one for each pair: $h_{ij} : \mathcal{X} \to \mathrm{R}$ for $i \in [1, k]$ and $j \in [i+1, k]$.
- Classifier h_{ij} distinguishes class i (+1) from class j (-1).

Prediction

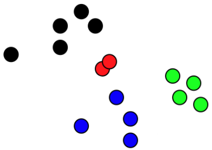
- Majority vote (each class gets $k-1$ votes)

$$h(x) = \underset{i \in \{1, \ldots, k\}}{\arg\max} \sum_{j \neq i} \underbrace{h_{ij}(x)\mathbb{I}\{i < j\}}_{\text{class } i \text{ is } +1} - \underbrace{h_{ji}(x)\mathbb{I}\{j < i\}}_{\text{class } i \text{ is -1}}$$

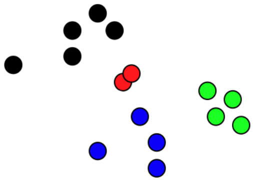
- Tournament
- Ties can be broken arbitrarily.

AvA: four-class example

Consider a dataset with four classes:

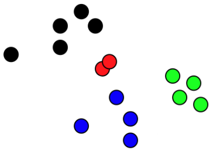


What's the decision region for the red class?



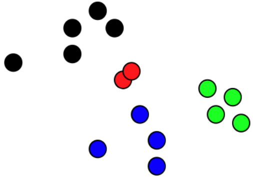
AvA: four-class example

Consider a dataset with four classes:



Assumption: each pair of classes are linearly separable.
More expressive than OvA.

What's the decision region for the red class?



OvA vs AvA

		OvA	AvA
computation	train	$O(k \quad)$	$O(k^2 \quad)$
	test	$O(k \quad)$	$O(k^2 \quad)$

OvA vs AvA

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$

challenges

OvA vs AvA

		OvA	AvA
computation	train	$O(kB_{\text{train}}(n))$	$O(k^2 B_{\text{train}}(n/k))$
	test	$O(kB_{\text{test}})$	$O(k^2 B_{\text{test}})$
challenges	train	class imbalance	small training set
	test	calibration / scale tie breaking	

Lack theoretical justification but simple to implement and works well in practice (when # classes is small).

Review

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- Key is to design "natural" binary classification problems without large computation cost.

Review

Reduction-based approaches:

- Reducing multiclass classification to binary classification: OvA, AvA
- Key is to design “natural” binary classification problems without large computation cost.

But,

- Unclear how to generalize to extremely large # of classes.
- ImageNet: >20k labels; Wikipedia: >1M categories.

Next, generalize previous algorithms to multiclass settings.

Multiclass Loss

Binary Logistic Regression

- Given an input x, we would like to output a classification between (0,1).

$$f(x) = sigmoid(z) = \frac{1}{1+\exp(-z)} = \frac{1}{1+\exp(-w^\top x - b)}. \tag{1}$$

Binary Logistic Regression

- Given an input x, we would like to output a classification between (0,1).

$$f(x) = sigmoid(z) = \frac{1}{1+\exp(-z)} = \frac{1}{1+\exp(-w^\top x - b)}. \tag{1}$$

- The other class is represented in $1 - f(x)$:

$$1 - f(x) = \frac{\exp(-w^\top x - b)}{1+\exp(-w^\top x - b)} = \frac{1}{1+\exp(w^\top x + b)} = sigmoid(-z). \tag{2}$$

Binary Logistic Regression

- Given an input x, we would like to output a classification between (0,1).

$$f(x) = sigmoid(z) = \frac{1}{1+\exp(-z)} = \frac{1}{1+\exp(-w^\top x - b)}. \tag{1}$$

- The other class is represented in $1 - f(x)$:

$$1 - f(x) = \frac{\exp(-w^\top x - b)}{1+\exp(-w^\top x - b)} = \frac{1}{1+\exp(w^\top x + b)} = sigmoid(-z). \tag{2}$$

- Another way to view: one class has $(+w, +b)$ and the other class has $(-w, -b)$.

Multi-class Logistic Regression

- Now what if we have one w_c for each class c?

Multi-class Logistic Regression

- Now what if we have one w_c for each class c?
- Also called "softmax" in neural networks.

Multi-class Logistic Regression

- Now what if we have one w_c for each class c?
- Also called "softmax" in neural networks.
- Loss function:

Multi-class Logistic Regression

- Now what if we have one w_c for each class c?
- Also called "softmax" in neural networks.
- Loss function:
- Gradient: $\frac{\partial L}{\partial z} = f - y$. Recall: MSE loss.

Comparison to OvA

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (score functions).
- **Multiclass Hypothesis Space** (for k classes):

$$\mathcal{F} = \left\{ x \mapsto \arg\max_i h_i(x) \mid h_1, \ldots, h_k \in \mathcal{H} \right\}$$

Comparison to OvA

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (score functions).
- **Multiclass Hypothesis Space** (for k classes):

$$\mathcal{F} = \left\{ x \mapsto \arg\max_i h_i(x) \mid h_1, \ldots, h_k \in \mathcal{H} \right\}$$

- Intuitively, $h_i(x)$ scores how likely x is to be from class i.
- OvA objective: $h_i(x) > 0$ for x with label i and $h_i(x) < 0$ for x with all other labels.

Comparison to OvA

- **Base Hypothesis Space**: $\mathcal{H} = \{h : \mathcal{X} \to \mathrm{R}\}$ (score functions).
- **Multiclass Hypothesis Space** (for k classes):

$$\mathcal{F} = \left\{ x \mapsto \arg\max_i h_i(x) \mid h_1, \ldots, h_k \in \mathcal{H} \right\}$$

- Intuitively, $h_i(x)$ scores how likely x is to be from class i.
- OvA objective: $h_i(x) > 0$ for x with label i and $h_i(x) < 0$ for x with all other labels.
- At test time, to predict (x, i) correctly we only need

$$h_i(x) > h_j(x) \qquad \forall j \neq i. \tag{3}$$

Multiclass Perceptron

- Base linear predictors: $h_i(x) = w_i^T x$ ($w \in \mathrm{R}^d$).

Multiclass Perceptron

- Base linear predictors: $h_i(x) = w_i^T x$ $(w \in \mathbb{R}^d)$.
- Multiclass perceptron:

Given a multiclass dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ **do**
  for $(x, y) \in \mathcal{D}$ **do**
    $\hat{y} = \arg\max_{y' \in \mathcal{Y}} w_{y'}^T x$;
    if $\hat{y} \neq y$ **then** `// We've made a mistake`
      $w_y \leftarrow w_y + x$; `// Move the target-class scorer towards` x
      $w_{\hat{y}} \leftarrow w_{\hat{y}} - x$; `// Move the wrong-class scorer away from` x
    end
  end
end

Rewrite the scoring function

- Remember that we want to scale to very large # of classes and reuse algorithms and analysis for binary classification
  - $\Longrightarrow$ a single weight vector is desired
- How to rewrite the equation such that we have one w instead of k?

Rewrite the scoring function

- Remember that we want to scale to very large # of classes and reuse algorithms and analysis for binary classification
  - $\implies$ a single weight vector is desired
- How to rewrite the equation such that we have one w instead of k?

$$w_i^T x = w^T \psi(x, i) \tag{4}$$

$$h_i(x) = h(x, i) \tag{5}$$

  - Encode labels in the feature space.
  - Score for each label $\rightarrow$ score for the "*compatibility*" of a label and an input.

The Multivector Construction

How to construct the feature map ψ?

The Multivector Construction

How to construct the feature map ψ?

- What if we stack w_i's together (e.g., $x \in \mathrm{R}^2, \mathcal{Y} = \{1,2,3\}$)

$$w = \Bigg(\underbrace{-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_1}, \underbrace{0, 1}_{w_2}, \underbrace{\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_3} \Bigg)$$

The Multivector Construction

How to construct the feature map ψ?

- What if we stack w_i's together (e.g., $x \in \mathbb{R}^2, \mathcal{Y} = \{1,2,3\}$)

$$w = \left(\underbrace{-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_1}, \underbrace{0, 1}_{w_2}, \underbrace{\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_3} \right)$$

- And then do the following: $\Psi : \mathbb{R}^2 \times \{1,2,3\} \to \mathbb{R}^6$ defined by

$$\begin{aligned} \Psi(x,1) &:= (x_1, x_2, 0, 0, 0, 0) \\ \Psi(x,2) &:= (0, 0, x_1, x_2, 0, 0) \\ \Psi(x,3) &:= (0, 0, 0, 0, x_1, x_2) \end{aligned}$$

The Multivector Construction

How to construct the feature map ψ?

- What if we stack w_i's together (e.g., $x \in \mathbb{R}^2, \mathcal{Y} = \{1,2,3\}$)

$$w = \left(\underbrace{-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_1}, \underbrace{0, 1}_{w_2}, \underbrace{\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}}_{w_3} \right)$$

- And then do the following: $\Psi : \mathbb{R}^2 \times \{1,2,3\} \to \mathbb{R}^6$ defined by

$$\begin{aligned} \Psi(x,1) &:= (x_1, x_2, 0, 0, 0, 0) \\ \Psi(x,2) &:= (0, 0, x_1, x_2, 0, 0) \\ \Psi(x,3) &:= (0, 0, 0, 0, x_1, x_2) \end{aligned}$$

- Then $\langle w, \Psi(x,y) \rangle = \langle w_y, x \rangle$, which is what we want.

Rewrite multiclass perceptron

Multiclass perceptron using the multivector construction.

```
Given a multiclass dataset 𝒟 = {(x, y)};
Initialize w ← 0;
for iter = 1, 2, ..., T do
    for (x, y) ∈ 𝒟 do
        ŷ = argmax_{y'∈𝒴} w^T ψ(x, y') ; // Equivalent to argmax_{y'∈𝒴} w_{y'}^T x
        if ŷ ≠ y then // We've made a mistake
            w ← w + ψ(x, y) ; // Move the scorer towards ψ(x, y)
            w ← w − ψ(x, ŷ) ; // Move the scorer away from ψ(x, ŷ)
        end
    end
end
```

Rewrite multiclass perceptron

Multiclass perceptron using the multivector construction.

Given a multiclass dataset $\mathcal{D} = \{(x, y)\}$;

Initialize $w \leftarrow 0$;

for $iter = 1, 2, \ldots, T$ **do**

  for $(x, y) \in \mathcal{D}$ **do**

    $\hat{y} = \arg\max_{y' \in \mathcal{Y}} w^T \psi(x, y')$; `// Equivalent to` $\arg\max_{y' \in \mathcal{Y}} w_{y'}^T x$

    if $\hat{y} \neq y$ **then** `// We've made a mistake`

      $w \leftarrow w + \psi(x, y)$; `// Move the scorer towards` $\psi(x, y)$

      $w \leftarrow w - \psi(x, \hat{y})$; `// Move the scorer away from` $\psi(x, \hat{y})$

    end

  end

end

Exercise: What is the base binary classification problem in multiclass perceptron?

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE,}\ldots\}$.

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN,VERB,ADJECTIVE,} \ldots\}$.
- Features of $x \in \mathcal{X}$: [The word itself], ENDS_IN_ly, ENDS_IN_ness, ...

How to construct the feature vector?

- Multivector construction: $w \in \mathbb{R}^{d \times k}$—doesn't scale.

Features

Toy multiclass example: Part-of-speech classification

- $\mathcal{X} = \{\text{All possible words}\}$
- $\mathcal{Y} = \{\text{NOUN}, \text{VERB}, \text{ADJECTIVE}, \ldots\}$.
- Features of $x \in \mathcal{X}$: [The word itself], ENDS_IN_ly, ENDS_IN_ness, ...

How to construct the feature vector?

- Multivector construction: $w \in \mathbb{R}^{d \times k}$—doesn't scale.
- Directly design features for each class.

$$\Psi(x, y) = (\psi_1(x, y), \psi_2(x, y), \psi_3(x, y), \ldots, \psi_d(x, y)) \tag{6}$$

  - Size can be bounded by d.

Features

Sample training data:

`The boy grabbed the apple and ran away quickly .`

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$
\begin{aligned}
\psi_1(x,y) &= \mathbb{1}[x = \text{apple AND } y = \text{NOUN}] \\
\psi_2(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{NOUN}] \\
\psi_3(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{VERB}] \\
\psi_4(x,y) &= \mathbb{1}[x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}] \\
&\ldots
\end{aligned}
$$

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$
\begin{aligned}
\psi_1(x,y) &= \mathbb{1}[x = \text{apple AND } y = \text{NOUN}] \\
\psi_2(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{NOUN}] \\
\psi_3(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{VERB}] \\
\psi_4(x,y) &= \mathbb{1}[x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}] \\
&\dots
\end{aligned}
$$

- E.g., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \dots)$

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$
\begin{aligned}
\psi_1(x,y) &= \mathbb{1}[x = \text{apple AND } y = \text{NOUN}] \\
\psi_2(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{NOUN}] \\
\psi_3(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{VERB}] \\
\psi_4(x,y) &= \mathbb{1}[x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}] \\
&\ldots
\end{aligned}
$$

- E.g., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \ldots)$
- After training, what's w_1, w_2, w_3, w_4?

Features

Sample training data:

```
The boy grabbed the apple and ran away quickly .
```

Feature:

$$
\begin{aligned}
\psi_1(x,y) &= \mathbb{1}[x = \text{apple AND } y = \text{NOUN}] \\
\psi_2(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{NOUN}] \\
\psi_3(x,y) &= \mathbb{1}[x = \text{run AND } y = \text{VERB}] \\
\psi_4(x,y) &= \mathbb{1}[x \text{ ENDS\_IN\_ly AND } y = \text{ADVERB}] \\
&\ldots
\end{aligned}
$$

- E.g., $\Psi(x = \text{run}, y = \text{NOUN}) = (0, 1, 0, 0, \ldots)$
- After training, what's w_1, w_2, w_3, w_4?
- No need to include features unseen in training data.

Feature templates: implementation

- Flexible, e.g., neighboring words, suffix/prefix.
- "Read off" features from the training data.
- Often sparse—efficient in practice, e.g., NLP problems.
- Can use a hash function: template $\rightarrow \{1, 2, \ldots, d\}$.

Review

Ingredients in multiclass classification:

- Scoring functions for each class (similar to ranking).
- Represent labels in the input space $\Longrightarrow$ single weight vector.

Review

Ingredients in multiclass classification:

- Scoring functions for each class (similar to ranking).
- Represent labels in the input space $\implies$ single weight vector.

We've seen

- How to generalize the perceptron algorithm to multiclass setting.
- Very simple idea. Was popular in NLP for structured prediction (e.g., tagging, parsing).

Review

Ingredients in multiclass classification:

- Scoring functions for each class (similar to ranking).
- Represent labels in the input space $\implies$ single weight vector.

We've seen

- How to generalize the perceptron algorithm to multiclass setting.
- Very simple idea. Was popular in NLP for structured prediction (e.g., tagging, parsing).

Next,

- How to generalize SVM to the multiclass setting.
- Concept check: Why might one prefer SVM / perceptron?

Margin for Multiclass

Binary

- Margin for $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{7}$$

- Want margin to be large and positive ($w^T x^{(n)}$ has same sign as $y^{(n)}$)

Margin for Multiclass

Binary

- Margin for $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{7}$$

- Want margin to be large and positive ($w^T x^{(n)}$ has same sign as $y^{(n)}$)

Multiclass

- Class-specific margin for $(x^{(n)}, y^{(n)})$:

$$h(x^{(n)}, y^{(n)}) - h(x^{(n)}, y). \tag{8}$$

- Difference between scores of the correct class and each other class
- Want margin to be large and positive for all $y \neq y^{(n)}$.

Multiclass SVM: separable case

Binary Recall binary formulation.

Multiclass SVM: separable case

Binary Recall binary formulation.

Multiclass As in the binary case, take 1 as our target margin.

Multiclass SVM: separable case

Binary Recall binary formulation.

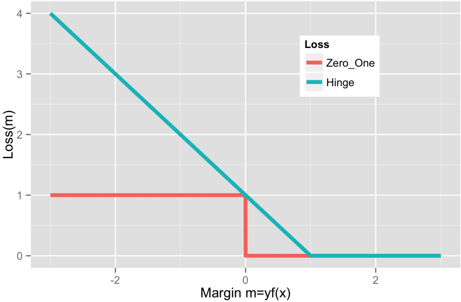
Multiclass As in the binary case, take 1 as our target margin.

Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

- Hinge loss: a convex upperbound on the 0-1 loss

$$\ell_{\text{hinge}}(y, \hat{y}) = \max(0, 1 - yh(x)) \tag{9}$$



Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$ \tag{10} $$

Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$\Delta(y, y') = \mathbb{I}\{y \neq y'\} \tag{10}$$

Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$\Delta(y, y') = \mathbb{I}\{y \neq y'\} \tag{10}$$

- In general, can also have different cost for each class.

Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$\Delta(y, y') = \mathbb{I}\{y \neq y'\} \tag{10}$$

- In general, can also have different cost for each class.
- Upper bound on $\Delta(y, y')$.

Generalized hinge loss

- What's the zero-one loss for multiclass classification?

$$\Delta(y, y') = \mathbb{I}\{y \neq y'\} \tag{10}$$

- In general, can also have different cost for each class.
- Upper bound on $\Delta(y, y')$.

- Generalized hinge loss:

Multiclass SVM with Hinge Loss

- Recall the hinge loss formulation for binary SVM (without the bias term):

Multiclass SVM with Hinge Loss

- Recall the hinge loss formulation for binary SVM (without the bias term):

- The multiclass objective:

  - $\Delta(y, y')$ as target margin for each class.
  - If margin $m_{n,y'}(w)$ meets or exceeds its target $\Delta(y^{(n)}, y')$ $\forall y \in \mathcal{Y}$, then no loss on example n.

Introduction to Structured Prediction

Example: Part-of-speech (POS) Tagging

- Given a sentence, give a part of speech tag for each word:

x	$\underbrace{\text{[START]}}_{x_0}$	$\underbrace{\text{He}}_{x_1}$	$\underbrace{\text{eats}}_{x_2}$	$\underbrace{\text{apples}}_{x_3}$
y	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

Example: Part-of-speech (POS) Tagging

- Given a sentence, give a part of speech tag for each word:

x	$\underbrace{\text{[START]}}_{x_0}$	$\underbrace{\text{He}}_{x_1}$	$\underbrace{\text{eats}}_{x_2}$	$\underbrace{\text{apples}}_{x_3}$
y	$\underbrace{\text{[START]}}_{y_0}$	$\underbrace{\text{Pronoun}}_{y_1}$	$\underbrace{\text{Verb}}_{y_2}$	$\underbrace{\text{Noun}}_{y_3}$

Example: Action grounding from long-form videos

- Given a long video, segment the video into short windows where each window corresponds to an action from a list of actions.
- E.g. slicing, chopping, frying, washing, etc.

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
  - Size depends on input x

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
  - Size depends on input x
- Base Hypothesis Space: $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}\}$
  - $h(x, y)$ gives compatibility score between input x and output y

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
  - Size depends on input x
- Base Hypothesis Space: $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}\}$
  - $h(x, y)$ gives compatibility score between input x and output y
- Multiclass hypothesis space

$$\mathcal{F} = \left\{ x \mapsto \underset{y \in \mathcal{Y}}{\arg\max}\, h(x, y) \mid h \in \mathcal{H} \right\}$$

- Final prediction function is an $f \in \mathcal{F}$.
- For each $f \in \mathcal{F}$ there is an underlying compatibility score function $h \in \mathcal{H}$.