

Data Science 4

Chris Mathys



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Decision Theory

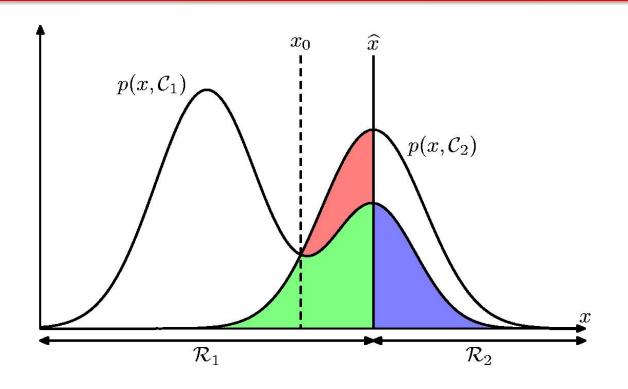
Inference step

Determine either $p(t|\mathbf{x})$ or $p(\mathbf{x},t)$.

Decision step

For given x, determine optimal t.

Minimum Misclassification Rate



$$p(\text{mistake}) = p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1)$$
$$= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) d\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) d\mathbf{x}.$$

Minimum Expected Loss

Example: classify medical images as 'cancer' or 'normal'

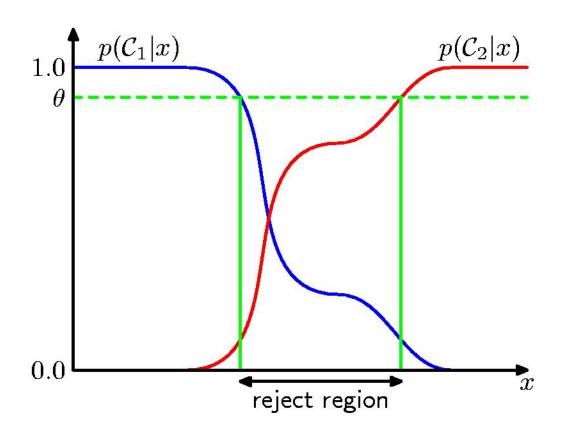
Minimum Expected Loss

$$\mathbb{E}[L] = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x}$$

Regions \mathcal{R}_j are chosen to minimize

$$\mathbb{E}[L] = \sum_{k} L_{kj} p(\mathcal{C}_k | \mathbf{x})$$

Reject Option



Why Separate Inference and Decision?

- Minimizing risk (loss matrix may change over time)
- Reject option
- Unbalanced class priors
- Combining models

Decision Theory for Regression

Inference step

Determine $p(\mathbf{x}, t)$.

Decision step

For given x, make optimal prediction, y(x), for t.

Loss function:
$$\mathbb{E}[L] = \iint L(t, y(\mathbf{x})) p(\mathbf{x}, t) d\mathbf{x} dt$$

The Squared Loss Function

$$\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) \, d\mathbf{x} \, dt$$

$$\{y(\mathbf{x}) - t\}^2 = \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}] + \mathbb{E}[t|\mathbf{x}] - t\}^2$$
$$= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\} + \{\mathbb{E}[t|\mathbf{x}] - t\}^2$$

$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 p(\mathbf{x}) d\mathbf{x} + \int \operatorname{var}[t|\mathbf{x}] p(\mathbf{x}) d\mathbf{x}$$

$$y(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}]$$

Generative vs Discriminative

Generative approach:

Model
$$p(t, \mathbf{x}) = p(\mathbf{x}|t)p(t)$$

Use Bayes' theorem $p(t|\mathbf{x}) = \frac{p(\mathbf{x}|t)p(t)}{p(\mathbf{x})}$

Discriminative approach:

Model $p(t|\mathbf{x})$ directly

$$H[x] = -\sum_{x} p(x) \log_2 p(x)$$

Important quantity in

- coding theory
- statistical physics
- machine learning

Coding theory: x discrete with 8 possible states; how many bits to transmit the state of x?

All states equally likely

$$H[x] = -8 \times \frac{1}{8} \log_2 \frac{1}{8} = 3 \text{ bits.}$$

$$H[x] = -\frac{1}{2}\log_2\frac{1}{2} - \frac{1}{4}\log_2\frac{1}{4} - \frac{1}{8}\log_2\frac{1}{8} - \frac{1}{16}\log_2\frac{1}{16} - \frac{4}{64}\log_2\frac{1}{64}$$
$$= 2 \text{ bits}$$

average code length =
$$\frac{1}{2} \times 1 + \frac{1}{4} \times 2 + \frac{1}{8} \times 3 + \frac{1}{16} \times 4 + 4 \times \frac{1}{64} \times 6$$

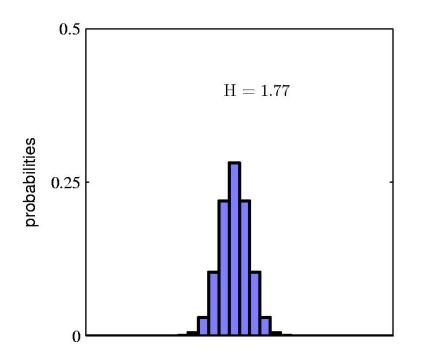
= 2 bits

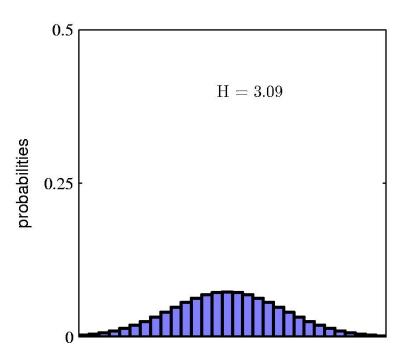
In how many ways can N identical objects be allocated M bins?

$$W = \frac{N!}{\prod_i n_i!}$$

$$H = \frac{1}{N} \ln W \simeq -\lim_{N \to \infty} \sum_{i} \left(\frac{n_i}{N}\right) \ln \left(\frac{n_i}{N}\right) = -\sum_{i} p_i \ln p_i$$

Entropy maximized when $\forall i: p_i = \frac{1}{M}$





Differential Entropy

Put bins of width ¢ along the real line

$$\lim_{\Delta \to 0} \left\{ -\sum_{i} p(x_i) \Delta \ln p(x_i) \right\} = -\int p(x) \ln p(x) dx$$

Differential entropy maximized (for fixed σ^2) when

$$p(x) = \mathcal{N}(x|\mu, \sigma^2)$$

in which case

$$H[x] = \frac{1}{2} \{1 + \ln(2\pi\sigma^2)\}.$$

Conditional Entropy

$$H[\mathbf{y}|\mathbf{x}] = -\iint p(\mathbf{y}, \mathbf{x}) \ln p(\mathbf{y}|\mathbf{x}) \, d\mathbf{y} \, d\mathbf{x}$$

$$H[\mathbf{x}, \mathbf{y}] = H[\mathbf{y}|\mathbf{x}] + H[\mathbf{x}]$$

The Kullback-Leibler Divergence

$$KL(p||q) = -\int p(\mathbf{x}) \ln q(\mathbf{x}) d\mathbf{x} - \left(-\int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}\right)$$
$$= -\int p(\mathbf{x}) \ln \left\{\frac{q(\mathbf{x})}{p(\mathbf{x})}\right\} d\mathbf{x}$$

$$\mathrm{KL}(p\|q) \simeq \frac{1}{N} \sum_{n=1}^{N} \left\{ -\ln q(\mathbf{x}_n|\boldsymbol{\theta}) + \ln p(\mathbf{x}_n) \right\}$$

$$KL(p||q) \geqslant 0$$
 $KL(p||q) \not\equiv KL(q||p)$

Mutual Information

$$I[\mathbf{x}, \mathbf{y}] \equiv KL(p(\mathbf{x}, \mathbf{y}) || p(\mathbf{x}) p(\mathbf{y}))$$

$$= -\iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x}) p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x} d\mathbf{y}$$

$$I[\mathbf{x}, \mathbf{y}] = H[\mathbf{x}] - H[\mathbf{x}|\mathbf{y}] = H[\mathbf{y}] - H[\mathbf{y}|\mathbf{x}]$$