MACHINE LEARNING: THEORETICAL CONCEPTS UE

Assignment 1: Maximum likelihood, Generalization Error

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Institute Homepage

Generalization Error

Supervised learning:

- some real world process produces data $\mathbf{x} \in \mathbb{R}^d$
- to every data point we want to infer a $y \in \mathbb{R}$ that is either a category (classification) or a value (regression)
- for a set of data points $X = \{\mathbf{x}^1, \dots, \mathbf{x}^l\}$ we know the associated $\{y^1, \dots, y^l\}$
- we call $\{\mathbf{z}^1, \dots, \mathbf{z}^l\}$ the training data, where $\mathbf{z}^i = (\mathbf{x}^i, y^i)$

What does it mean to learn from data?

- learning is model selection
- supervised learning: select a model that minimizes the prediction error on future data
- i.e. we want our model to generalize from the training data to future data

Generalization Error

What does it mean to learn from data? More formal:

- selecting a model, i.e. a function $g(\mathbf{x})$ that associates y to input $\mathbf{x}$
- if the model is parametrized with an vector $\mathbf{w}$ we write $g(\mathbf{x};\mathbf{w})$
- we want to select a "good" model (i.e. good parameters)
- we measure the performance of our model with a loss function $L(y, g(\mathbf{x};\mathbf{w}))$

Typical loss functions

- zero-one-loss

  $$L(y, g(\mathbf{x};\omega)) = \begin{cases} 0 & \text{for } y = g(\mathbf{x};\omega) \\ 1 & \text{for } y \neq g(\mathbf{x};\omega) \end{cases}$$

- quadratic loss

  $$L(y, g(\mathbf{x};\omega)) = (y - g(\mathbf{x};\omega))^2$$

Generalization Error

What does it mean to generalize?

- the **generalization error** which is the **expected loss on future data** should be as low as possible
- the generalization error, also called the risk R is the functional:

$$R(g(.;\mathbf{w})) \; = \; E_{\mathbf{z}}\left(L(y, g(\mathbf{x};\mathbf{w}))\right) = \int_Z L(y, g(\mathbf{x};\mathbf{w}))\; p(\mathbf{z})\; d\mathbf{z}$$

where $p(\mathbf{z})$ denotes the probability of $\mathbf{z}$ and Z is the set of all future $\mathbf{z}$.

Since we don't have all future data, we need to approximate the risk

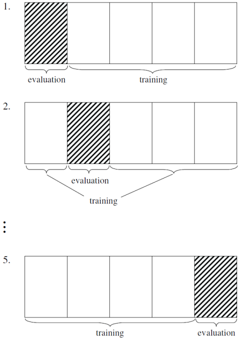
- we choose m samples from $\{\mathbf{z}^1, \ldots, \mathbf{z}^l\ \}$
- this is the so called "test set" $\{\mathbf{z}^1, \ldots, \mathbf{z}^m\ \}$, $m < l$
- assuming the $\mathbf{z}$ are iid and m is large enough we can approximate the risk

$$R(g(.;\mathbf{w})) \approx \frac{1}{m} \sum_{i=1}^{m} \left(L(y^i, g(\mathbf{x}^i;\mathbf{w}))\right)$$

Empirical Estimation of Risk

If we don’t have much data:

- Cross Validation: using folds of the data



CV risk is an almost unbiased estimator for the risk

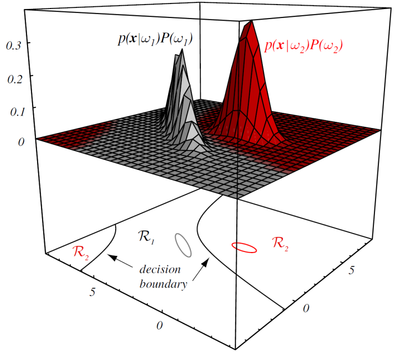
Minimal Risk for Gaussian Classification

Density function of multivariate Gaussian:

$$\mathcal{N}(\mathbf{x}; \mu, \mathbf{\Sigma}) = \frac{1}{(2\,\pi)^{d/2}\,|\mathbf{\Sigma}|^{1/2}}\; e^{-\frac{1}{2}\,(\mathbf{x}-\mu)^T\,\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)}$$

Classification task where the data for each class is drawn from a Gaussian

- $p(\mathbf{x}|y=1) \propto \mathcal{N}(\mu_1, \mathbf{\Sigma}_1)$
- $p(\mathbf{x}|y=-1) \propto \mathcal{N}(\mu_{-1}, \mathbf{\Sigma}_{-1})$



A two-dimensional classification task where the data for each class are drawn from a Gaussian (black: class 1, red: class -1). The optimal decision boundaries are two hyperbolas. Here $\omega_1 \equiv y = 1$ and $\omega_2 \equiv y = -1$. In the gray regions $p(y = 1 \mid \mathbf{x}) > p(y = -1 \mid \mathbf{x})$ holds and in the red regions the opposite holds. Copyright © 2001 John Wiley & Sons, Inc.

Minimal Risk for Gaussian Classification

We define the regions

- of class 1 as $X_1 \; = \; \{\mathbf{x} \mid g(\mathbf{x}) > 0\}$
- of class -1 as $X_{-1} \; = \; \{\mathbf{x} \mid g(\mathbf{x}) < 0\}$

and the loss function as

$$L(y, g(\mathbf{x};\omega)) \;=\; \begin{cases} 0 & \text{for} \quad y \cdot g(\mathbf{x};\omega) > 0 \\ 1 & \text{for} \quad y \cdot g(\mathbf{x};\omega) < 0 \end{cases}$$

Using the zero-one-loss we obtain for the risk

$$\begin{aligned} R(g(.;\omega)) &= \int_{X_1} p\,(y=-1 \mid \mathbf{x})\; p(\mathbf{x})\; d\mathbf{x} \;+\; \int_{X_{-1}} p\,(y=1 \mid \mathbf{x})\; p(\mathbf{x})\; d\mathbf{x} \\ &= \int_X \left\{ \begin{array}{lll} p\,(y=-1 \mid \mathbf{x}) & \text{for} & g(\mathbf{x}) > 0 \\ p\,(y=1 \mid \mathbf{x}) & \text{for} & g(\mathbf{x}) < 0 \end{array} \right\} p(\mathbf{x})\; d\mathbf{x}\,. \end{aligned}$$

Minimal Risk for Gaussian Classification

Risk can be minimized by

- choosing the smaller value of $p\,(y=-1 \mid \mathbf{x})$ and $p\,(y=1 \mid \mathbf{x})$.

Therefore, risk is minimal if

$$g(\mathbf{x};\omega) \begin{cases} >\ 0 & \text{for} \quad p\,(y=1 \mid \mathbf{x})\ >\ p\,(y=-1 \mid \mathbf{x}) \\ <\ 0 & \text{for} \quad p\,(y=-1 \mid \mathbf{x})\ >\ p\,(y=1 \mid \mathbf{x}) \end{cases}$$

The minimal risk is

$$R_{\min} = \int_X \min\{p\,(y=-1 \mid \mathbf{x})\,, p\,(y=1 \mid \mathbf{x})\}\ p(\mathbf{x})\ d\mathbf{x}$$

Discriminant Function

A discriminant function which minimizes the future risk is

$$\begin{aligned} g(\mathbf{x}) &= \; p(y=1 \mid \mathbf{x}) \; - \; p(y=-1 \mid \mathbf{x}) \\ &= \frac{1}{p(\mathbf{x})} \left(\, p(\mathbf{x} \mid y=1) \, p(y=1) \; - \; p(\mathbf{x} \mid y=-1) \, p(y=-1) \, \right) \; , \end{aligned}$$

- only the difference in the last brackets matters because $p(\mathbf{x}) > 0$
- optimal discriminant function is not unique since difference of strict monotone mappings of $p(y=1 \mid \mathbf{x})$ and $p(y=-1 \mid \mathbf{x})$ keep the sign

Take the logarithm → more convenient discriminant function which also minimizes the future risk:

$$\begin{aligned} g(\mathbf{x}) &= \ln p(y=1 \mid \mathbf{x}) \; - \; \ln p(y=-1 \mid \mathbf{x}) \\ &= \ln \frac{p(\mathbf{x} \mid y=1)}{p(\mathbf{x} \mid y=-1)} \; + \; \ln \frac{p(y=1)}{p(y=-1)} \; . \end{aligned}$$

Discriminant Function for Gaussian Classific.

$$
\begin{aligned}
g(\mathbf{x}) &= -\frac{1}{2}\,(\mathbf{x}-\mu_1)^T\,\mathbf{\Sigma}_1^{-1}(\mathbf{x}-\mu_1) \;-\; \frac{d}{2}\ln 2\pi \;-\; \frac{1}{2}\,\ln|\mathbf{\Sigma}_1| \;+\ln p(y=1) \\
&\quad +\frac{1}{2}\,(\mathbf{x}-\mu_{-1})^T\,\mathbf{\Sigma}_{-1}^{-1}(\mathbf{x}-\mu_{-1}) + \;\frac{d}{2}\ln 2\pi \;+\; \frac{1}{2}\,\ln|\mathbf{\Sigma}_{-1}| \;-\; \ln p(y=-1) \\
&= -\frac{1}{2}\,(\mathbf{x}-\mu_1)^T\,\mathbf{\Sigma}_1^{-1}(\mathbf{x}-\mu_1) \;-\; \frac{1}{2}\,\ln|\mathbf{\Sigma}_1| \;+\; \ln p(y=1) \\
&\quad +\frac{1}{2}\,(\mathbf{x}-\mu_{-1})^T\,\mathbf{\Sigma}_{-1}^{-1}(\mathbf{x}-\mu_{-1}) \;+\; \frac{1}{2}\,\ln|\mathbf{\Sigma}_{-1}| \;-\; \ln p(y=-1) \\
&= -\frac{1}{2}\mathbf{x}^T\left(\mathbf{\Sigma}_1^{-1} \;-\; \mathbf{\Sigma}_{-1}^{-1}\right)\,\mathbf{x} \;+\; \mathbf{x}^T\left(\mathbf{\Sigma}_1^{-1}\mu_1 \;-\; \mathbf{\Sigma}_{-1}^{-1}\mu_{-1}\right) \;-\; \frac{1}{2}\,\mu_1^T\mathbf{\Sigma}_1^{-1}\mu_1 \\
&\quad +\frac{1}{2}\,\mu_{-1}^T\mathbf{\Sigma}_{-1}^{-1}\mu_{-1} \;-\; \frac{1}{2}\,\ln|\mathbf{\Sigma}_1| \;+\; \frac{1}{2}\,\ln|\mathbf{\Sigma}_{-1}| \;+\ln p(y=1) \;-\; \ln p(y=-1) \\
&= -\frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} \;+\; \mathbf{w}^T\mathbf{x} \;+\; b\,.
\end{aligned}
$$

Maximum Likelihood

Quality criterion for our model:

- in case of supervised learning: generalization error
- in case of unsupervised learning: Maximum Likelihood

Unsupervised setting:

- **Given:**
  - □ data samples $\{\mathbf{x}\} = \{\mathbf{x}^1, \ldots, \mathbf{x}^l\}$ (note: here $\mathbf{z}^i = \mathbf{x}^i$, i.e. no labels!)
  - □ a parametrized model distribution $p(\mathbf{x}; \hat{\mathbf{w}})$ where $\hat{\mathbf{w}}$ are the parameters
- **Task:** find the parameter $\mathbf{w}$ that was most likely to produce this data.
- **Idea:** How likely was a given $\hat{\mathbf{w}}$ to produce the dataset? Assuming that the $\mathbf{x}$ are iid.:

$$\mathcal{L}(\{\mathbf{x}\}; \hat{\mathbf{w}}) = p(\{\mathbf{x}\}; \hat{\mathbf{w}}) = \prod_{i=1}^{n} p(\mathbf{x}^i; \hat{\mathbf{w}})$$

- **Solution:** Find the $\mathbf{w}^*$ that maximizes $\mathcal{L}(\{\mathbf{x}\}; \hat{\mathbf{w}})$

Maximum Likelihood

Find the $\mathbf{w}^*$ that maximizes $\mathcal{L}(\{\mathbf{x}\}; \hat{\mathbf{w}})$:

$$\mathbf{w}^* = \underset{\hat{\mathbf{w}}}{arg\ max}\ \mathcal{L}(\{\mathbf{x}\}; \hat{\mathbf{w}}) = \underset{\hat{\mathbf{w}}}{arg\ max} \prod_{i=1}^{n} p(\mathbf{x}^i; \hat{\mathbf{w}})$$

It is better to optimize a sum instead of a product: log trick!

$$\mathbf{w}^* = \underset{\hat{\mathbf{w}}}{arg\ max}\ log\ \mathcal{L}(\{\mathbf{x}\}; \hat{\mathbf{w}}) = \underset{\hat{\mathbf{w}}}{arg\ max} \sum_{i=1}^{n} log\ p(\mathbf{x}^i; \hat{\mathbf{w}})$$