Machine Intelligence 2

5.1 Probability Density Estimation

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SS 2017

Density estimation

Density estimation is relevant

If p(x) is known, all predictable quantities can be deduced (mean, variance, higher order moments, p(x in interval)...

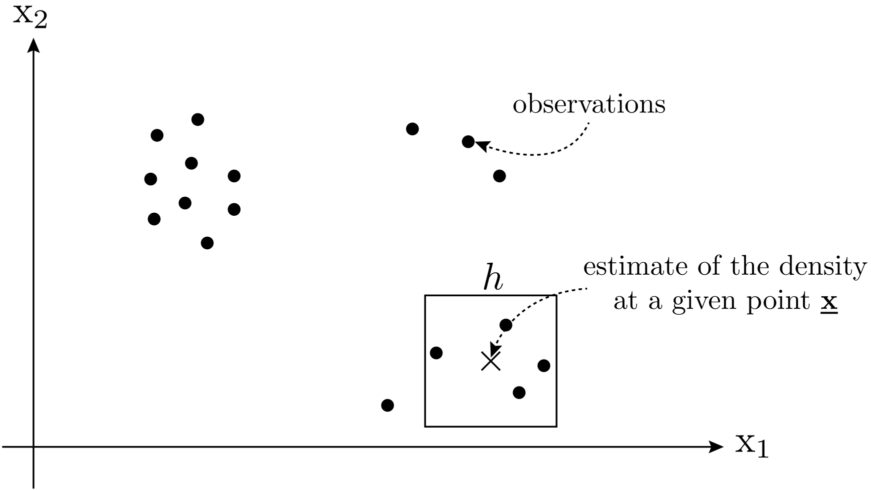
Density estimation is difficult (without prior knowledge)

How can we estimate the density for each possible outcome?

2 strategies:

1. **parametric** methods: model-based (e.g. Gaussian densities)
2. **nonparametric** methods: data driven (cf. Kernel density estimate)

(Nonparametric) Kernel density estimation



"Gliding histograms"

Count the number of data points within a volume V centered on $\underline{\mathbf{x}}$.

Histogram kernel:

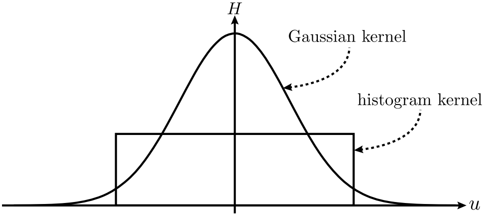
$$H(\underline{\mathbf{u}}) = \begin{cases} 1, & |u_j| < \frac{1}{2}, \forall j \in 1, \ldots, n \\ 0, & \text{else} \end{cases}$$

Density estimate ("gliding histogram"):

$$\widehat{P}(\underline{\mathbf{x}}) = \underbrace{\frac{1}{h^n}}_{\substack{\text{normalization} \\ \text{("density"!)}}} \cdot \underbrace{\frac{1}{p} \overbrace{\sum_{\alpha=1}^{p} H\left(\frac{\underline{\mathbf{x}} - \underline{\mathbf{x}}^{(\alpha)}}{h}\right)}^{\substack{\text{number of data points} \\ \text{within volume } V \text{ around } \underline{\mathbf{x}}}}}_{\text{fraction of data points}}$$

Histogram kernels lead to discontinuous pdf estimates $\rightsquigarrow$ use other kernels for smooth pdf estimates.

Gaussian kernels



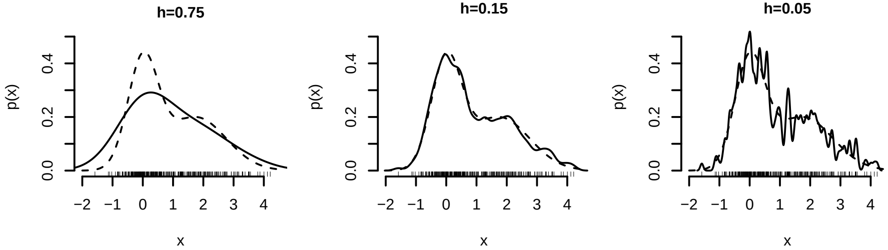
Gaussian kernel:

$$H(\underline{\mathbf{u}}) = \frac{1}{(2\pi)^{\frac{n}{2}}} \exp\left(- \frac{\underline{\mathbf{u}}^2}{2} \right)$$

Density estimate:

$$\begin{aligned} \widehat{P}(\underline{\mathbf{x}}) &= \frac{1}{h^n} \cdot \frac{1}{p} \sum_{\alpha=1}^{p} H\left(\frac{\underline{\mathbf{x}} - \underline{\mathbf{x}}^{(\alpha)}}{h} \right) \\ &= \frac{1}{p} \sum_{\alpha=1}^{p} \frac{1}{\left(2\pi h^2\right)^{\frac{n}{2}}} \exp\left\{ - \frac{\left(\underline{\mathbf{x}} - \underline{\mathbf{x}}^{(\alpha)}\right)^2}{2h^2} \right\} \end{aligned}$$

Effects of kernel width



Choice of kernel width $\Rightarrow$ model selection / validation

Parametric density estimation

observations: $\left\{\underline{\mathbf{x}}^{(\alpha)}\right\}, \alpha = 1, \ldots, p$
parametrized family of pdfs: $\widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}}) \leftarrow$ "generative model"

example: multivariate Gaussian

$$\widehat{P}(\underline{\mathbf{x}}; \overbrace{\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\Sigma}}}^{\underline{\mathbf{w}}}) = \underbrace{\frac{1}{\sqrt{(2\pi)^N \det \underline{\boldsymbol{\Sigma}}}} \exp\left(-\frac{1}{2}(\underline{\mathbf{x}} - \underline{\boldsymbol{\mu}})^T \underline{\boldsymbol{\Sigma}}^{-1} (\underline{\mathbf{x}} - \underline{\boldsymbol{\mu}})\right)}_{\mathcal{N}(\underline{\mathbf{x}}; \underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\Sigma}})}$$

comment

here: $\widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}})$ for unconditional densities $P(\underline{\mathbf{x}}) \Rightarrow$ unsupervised learning
MI I: $\widehat{P}(y|\underline{\mathbf{x}}; \underline{\mathbf{w}})$ for conditional densities $P(y|\underline{\mathbf{x}}) \Rightarrow$ supervised learning

$\Rightarrow$ model Selection

Parametric density estimation

Generative model: parametrized family of pdfs: $\widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}})$

Model selection

Select the model (set of parameters) which is most similar to the true density!

Kullback-Leibler-Divergence

$$\mathrm{D}_{\mathrm{KL}}\Big[P(\underline{\mathbf{x}}), \widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}})\Big] = \int d\underline{\mathbf{x}} P(\underline{\mathbf{x}}) \ln \frac{P(\underline{\mathbf{x}})}{\widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}})} \overset{!}{=} \min_{(\underline{\mathbf{w}})}$$

- $\mathrm{D}_{\mathrm{KL}} \geq 0$ and $\mathrm{D}_{\mathrm{KL}} = 0$ iff $\widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}}) = P(\underline{\mathbf{x}})$
- distance measure between probability distributions

Model selection via Empirical Risk Minimization

$$\mathrm{D_{KL}}(P, \hat{P}_{\underline{\mathbf{w}}}) \stackrel{!}{=} \min_{(\underline{\mathbf{w}})}$$

$$\begin{aligned}
\underline{\mathbf{w}}^* \quad &= \operatorname*{argmin}_{(\underline{\mathbf{w}})} \left\{ \int d\underline{\mathbf{x}} P(\underline{\mathbf{x}}) \ln P(\underline{\mathbf{x}}) - \int d\underline{\mathbf{x}} P(\underline{\mathbf{x}}) \ln \widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}}) \right\} \\
&= \operatorname*{argmin}_{(\underline{\mathbf{w}})} \left\{ \underbrace{- \int d\underline{\mathbf{x}} P(\underline{\mathbf{x}}) \ln \widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}})}_{E^G_{[\underline{\mathbf{w}}]}} \right\}
\end{aligned}$$

"cross entropy"

$$E^G \stackrel{!}{=} \min_{(\underline{\mathbf{w}})}$$

Problem: $P(\underline{\mathbf{x}})$ is unknown.

Model selection via Empirical Risk Minimization

$$\boxed{\text{mathematical expectation } E^G} \longrightarrow \boxed{\text{empirical average } E^T}$$

"generalization cost" "training cost"

cost function:

$$E^T = -\frac{1}{p}\sum_{\alpha=1}^{p} \ln \widehat{P}\big(\underline{\mathbf{x}}^{(\alpha)}; \underline{\mathbf{w}}\big)$$

When is this a reasonable procedure? $\rightsquigarrow$ statistical learning theory *(MI I)*

criterion for model selection

$$\boxed{E^T = -\tfrac{1}{p}\sum_{\alpha=1}^{p} \ln \widehat{P}\big(\underline{\mathbf{x}}^{(\alpha)}; \underline{\mathbf{w}}\big) \stackrel{!}{=} \min_{(\underline{\mathbf{w}})}}$$

Optimization of the empirical risk

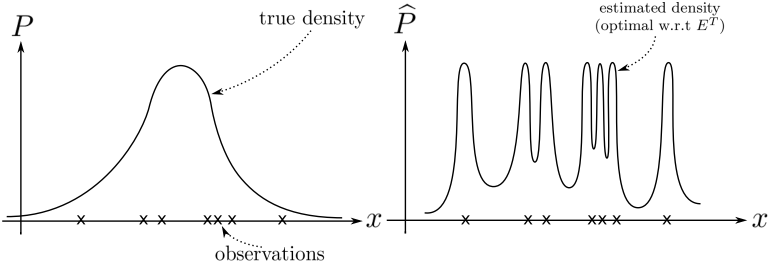
$$\underbrace{E^T_{[\underline{\mathbf{w}}]}}_{\substack{\text{total}\\\text{cost}}} = -\frac{1}{p}\sum_{\alpha=1}^{p} \ln \widehat{P}\big(\underline{\mathbf{x}}^{(\alpha)}; \underline{\mathbf{w}}\big) = \frac{1}{p}\sum_{\alpha=1}^{p} \underbrace{e^{(\alpha)}_{[\underline{\mathbf{w}}]}}_{\substack{\text{individual}\\\text{cost}}}$$

standard procedures e.g. (stochastic) gradient descent – cf. MI I

$$\left.\begin{array}{ll} \text{"batch"-learning:} & \Delta\underline{\mathbf{w}} = -\varepsilon\frac{\partial E^T}{\partial\underline{\mathbf{w}}} \\[2em] \text{"on-line"-learning:} & \Delta\underline{\mathbf{w}} = -\varepsilon\frac{\partial e^{(\alpha)}}{\partial\underline{\mathbf{w}}} \end{array}\right\} \begin{array}{c}\text{examples for}\\\text{gradient-based}\\\text{methods}\end{array}$$

Validation

Minimized training cost underestimates the corresponding generalization cost



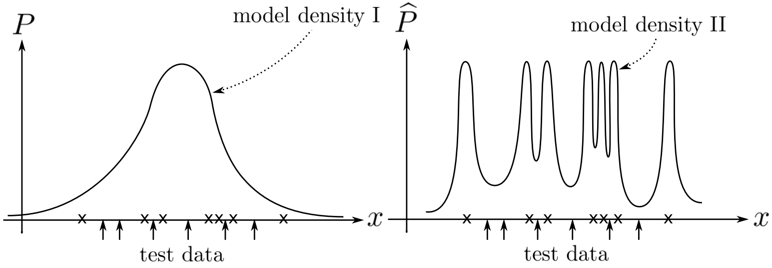
Overfitting:
E^T small but E^G large $\Rightarrow$ test-set method, n-fold cross-validation

Test-set method

$$\text{observations:} \begin{cases} \text{training data} & \{\underline{\mathbf{x}}^{(\alpha)}\}, \alpha = 1, \ldots, p \\ \\ \text{test data} & \{\underline{\mathbf{x}}^{(\beta)}\}, \beta = 1, \ldots, q \end{cases}$$

$$\widehat{E}^G = \frac{1}{q} \sum_{\beta=1}^{q} e^{(\beta)} \leftarrow \text{ estimate of } E^G$$

Test-set method



- $E^T_{(I)} > E^T_{(II)}$ but $E^G_{(I)} << E^G_{(II)}$
- Alternative method: **n-fold cross-validation** *(MI I)*

Comment

Validation methods are essential for estimating hyperparameters for non-parametric methods (e.g. Kernel density estimate).

The likelihood function

generative model

$\widehat{P}(\underline{\mathbf{x}}; \underline{\mathbf{w}})$ probability density for the generation of one data point

likelihood of the model = p(observations given the model)

assuming iid. observations:

$$\widehat{P}\big(\{\underline{\mathbf{x}}^{(\alpha)}\}; \underline{\mathbf{w}}\big) = \prod_{\alpha=1}^{p} \widehat{P}\big(\underline{\mathbf{x}}^{(\alpha)}; \underline{\mathbf{w}}\big)$$

Model selection and Maximum Likelihood

$$\widehat{P}\big(\{\underline{\mathbf{x}}^{(\alpha)}\}; \underline{\mathbf{w}}\big) \overset{!}{=} \max_{(\underline{\mathbf{w}})}$$

intuition: select the model which generates the observed data with high probability

in practice: minimization of the negative $\log$-likelihood

$$\begin{aligned} p \cdot E^T_{[\underline{\mathbf{w}}]} &= -\ln \widehat{P}\big(\{\underline{\mathbf{x}}^{(\alpha)}\}; \underline{\mathbf{w}}\big) \\ &= -\sum_{\alpha=1}^{p} \ln \widehat{P}\big(\underline{\mathbf{x}}^{(\alpha)}; \underline{\mathbf{w}}\big) \\ &\overset{!}{=} \min \end{aligned}$$

- equivalent to the minimization of the KL-divergence via ERM.

The multivariate Gaussian

$$\widehat{P}\left(\left\{\underline{\mathbf{x}}^{(\alpha)}\right\};\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\Sigma}}\right)=\left(\frac{1}{\sqrt{(2\pi)^N\det\underline{\boldsymbol{\Sigma}}}}\right)^p\cdot\prod_{\alpha=1}^{p}\exp\left(-\frac{1}{2}\left(\underline{\mathbf{x}}^{(\alpha)}-\underline{\boldsymbol{\mu}}\right)^T\underline{\boldsymbol{\Sigma}}^{-1}\left(\underline{\mathbf{x}}^{(\alpha)}-\underline{\boldsymbol{\mu}}\right)\right)$$

$$\begin{aligned}E^T\left(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\Sigma}}\right) &= -\ln\widehat{P}\left(\left\{\underline{\mathbf{x}}^{(\alpha)}\right\};\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\Sigma}}\right)\\ &= \frac{p\cdot N}{2}\ln(2\pi)+\frac{p}{2}\ln(\det\underline{\boldsymbol{\Sigma}})+\frac{1}{2}\sum_{\alpha=1}^{p}\left(\underline{\mathbf{x}}^{(\alpha)}-\underline{\boldsymbol{\mu}}\right)^T\underline{\boldsymbol{\Sigma}}^{-1}\left(\underline{\mathbf{x}}^{(\alpha)}-\underline{\boldsymbol{\mu}}\right)\end{aligned}$$

minimization of E^T (necessary conditions):

$$\frac{\partial E^T}{\partial\underline{\boldsymbol{\mu}}}=\underline{\mathbf{0}}\quad\Rightarrow\quad\underline{\boldsymbol{\mu}}^*=\frac{1}{p}\sum_{\alpha=1}^{p}\underline{\mathbf{x}}^{(\alpha)}\qquad\text{(empirical average)}$$

$$\frac{\partial E^T}{\partial\underline{\boldsymbol{\Sigma}}}=\underline{\mathbf{0}}\quad\Rightarrow\quad\underline{\boldsymbol{\Sigma}}^*=\frac{1}{p}\sum_{\alpha=1}^{p}(\underline{\mathbf{x}}^{(\alpha)}-\underline{\boldsymbol{\mu}}^*)(\underline{\mathbf{x}}^{(\alpha)}-\underline{\boldsymbol{\mu}}^*)^T\qquad\text{(empirical covariance matrix)}$$

remark: $\underline{\boldsymbol{\mu}}^*$ is unbiased, but $\underline{\boldsymbol{\Sigma}}^*$ is a biased estimator (cf. section: 6.1 Model fitting)