Estimating Unnormalised Models by Score Matching

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Program

1. Basics of score matching
2. Practical objective function for score matching

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1. Basics of score matching
   - Basic ideas of score matching
   - Objective function that captures the basic ideas but cannot be computed

2. Practical objective function for score matching

Problem formulation

- We want to estimate the parameters $\boldsymbol{\theta}$ of a parametric statistical model for a random vector $\mathbf{x} \in \mathbb{R}^d$.
- Given: iid data $\mathbf{x}_i, \ldots, \mathbf{x}_n$ that are assumed to be observations of $\mathbf{x}$ that has pdf p_*
- Further notation: $p(\boldsymbol{\xi}; \boldsymbol{\theta})$ is the model pdf; $\boldsymbol{\xi} \in \mathbb{R}^d$ is a dummy variable.
- Assumptions:
  - Model $p(\boldsymbol{\xi}; \boldsymbol{\theta})$ is known only up the partition function

$$p(\boldsymbol{\xi}; \boldsymbol{\theta}) = \frac{\tilde{p}(\boldsymbol{\xi}; \boldsymbol{\theta})}{Z(\boldsymbol{\theta})} \qquad Z(\boldsymbol{\theta}) = \int_{\boldsymbol{\xi}} \tilde{p}(\boldsymbol{\xi}; \boldsymbol{\theta}) \mathrm{d}\boldsymbol{\xi}$$

  - Functional form of $\tilde{p}$ is known (can be easily computed)
  - Partition function $Z(\boldsymbol{\theta})$ cannot be computed analytically in closed form and numerical approximation is expensive.
- Goal: Estimate the model without approximating the partition function $\mathbf{Z}(\boldsymbol{\theta})$.

Basic ideas of score matching

- Maximum likelihood estimation can be considered to find parameter values $\hat{\boldsymbol{\theta}}$ so that

$$p(\boldsymbol{\xi};\hat{\boldsymbol{\theta}}) \approx p_*(\boldsymbol{\xi}) \qquad \text{or} \qquad \log p(\boldsymbol{\xi};\hat{\boldsymbol{\theta}}) \approx \log p_*(\boldsymbol{\xi})$$

(as measured by Kullback-Leibler divergence, see Barber 8.7)

- Instead of estimating the parameters $\boldsymbol{\theta}$ by matching (log) densities, score matching identifies parameter values $\hat{\boldsymbol{\theta}}$ for which the derivatives (slopes) of the log densities match

$$\nabla_{\boldsymbol{\xi}} \log p(\boldsymbol{\xi};\hat{\boldsymbol{\theta}}) \approx \nabla_{\boldsymbol{\xi}} \log p_*(\boldsymbol{\xi})$$

- $\nabla_{\boldsymbol{\xi}} \log p(\boldsymbol{\xi};\boldsymbol{\theta})$ does not depend on the partition function:

$$\nabla_{\boldsymbol{\xi}} \log p(\boldsymbol{\xi};\boldsymbol{\theta}) = \nabla_{\boldsymbol{\xi}} \left[\log \tilde{p}(\boldsymbol{\xi};\boldsymbol{\theta}) - \log Z(\boldsymbol{\theta})\right] = \nabla_{\boldsymbol{\xi}} \log \tilde{p}(\boldsymbol{\xi};\boldsymbol{\theta})$$

The score function (in the context of score matching)

- Define the model score function $\mathbb{R}^d \to \mathbb{R}^d$ as

$$\boldsymbol{\psi}(\boldsymbol{\xi};\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial \log p(\boldsymbol{\xi};\boldsymbol{\theta})}{\partial \xi_1} \\ \vdots \\ \frac{\partial \log p(\boldsymbol{\xi};\boldsymbol{\theta})}{\partial \xi_d} \end{pmatrix} = \nabla_{\boldsymbol{\xi}} \log p(\boldsymbol{\xi};\boldsymbol{\theta})$$

  While defined in terms of $p(\boldsymbol{\xi};\boldsymbol{\theta})$, we also have

$$\boldsymbol{\psi}(\boldsymbol{\xi};\boldsymbol{\theta}) = \nabla_{\boldsymbol{\xi}} \log \tilde{p}(\boldsymbol{\xi};\boldsymbol{\theta})$$

- Similarly, define the data score function as

$$\boldsymbol{\psi}_*(\boldsymbol{\xi}) = \nabla_{\boldsymbol{\xi}} \log p_*(\boldsymbol{\xi})$$

Definition of the SM objective function

- Estimate $\boldsymbol{\theta}$ by minimising a distance between model score function $\boldsymbol{\psi}(\boldsymbol{\xi};\boldsymbol{\theta})$ and score function of observed data $\boldsymbol{\psi}_*(\boldsymbol{\xi})$

$$
\begin{aligned}
J_{\mathrm{sm}}(\boldsymbol{\theta}) &= \frac{1}{2}\int_{\boldsymbol{\xi}\in\mathbb{R}^m} p_*(\boldsymbol{\xi})\|\boldsymbol{\psi}(\boldsymbol{\xi};\boldsymbol{\theta}) - \boldsymbol{\psi}_*(\boldsymbol{\xi})\|^2 d\boldsymbol{\xi} \\
&= \frac{1}{2}\mathbb{E}_*\|\boldsymbol{\psi}(\mathbf{x};\boldsymbol{\theta}) - \boldsymbol{\psi}_*(\mathbf{x})\|^2 \qquad (\mathbf{x}\sim p_*)
\end{aligned}
$$

- Since $\boldsymbol{\psi}(\boldsymbol{\xi};\boldsymbol{\theta}) = \nabla_{\boldsymbol{\xi}} \log \tilde{p}(\boldsymbol{\xi};\boldsymbol{\theta})$ does not depend on $Z(\boldsymbol{\theta})$ there is no need to compute the partition function.
- Knowing the unnormalised model $\tilde{p}(\boldsymbol{\xi};\boldsymbol{\theta})$ is enough.
- Expectation $\mathbb{E}_*$ with respect to p_* can be approximated as sample average over the observed data, but what about $\boldsymbol{\psi}_*$?

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    - Integration by parts to obtain a computable objective function
    - Simple example

Reformulation of the SM objective function

- In the objective function we have the score function of the data distribution $\boldsymbol{\psi}_*$. How to compute it?
- In fact, no need to compute it because the score matching objective function J_{sm} can be expressed as

$$J_{\mathrm{sm}}(\boldsymbol{\theta}) = \mathbb{E}_* \sum_{j=1}^{d} \left[\partial_j \psi_j(\mathbf{x}; \boldsymbol{\theta}) + \frac{1}{2} \psi_j^2(\mathbf{x}; \boldsymbol{\theta}) \right] + \text{const.}$$

where the constant does not depend on $\boldsymbol{\theta}$, and

$$\psi_j(\boldsymbol{\xi}; \boldsymbol{\theta}) = \frac{\partial \log \tilde{p}(\boldsymbol{\xi}; \boldsymbol{\theta})}{\partial \xi_j} \qquad \partial_j \psi_j(\boldsymbol{\xi}; \boldsymbol{\theta}) = \frac{\partial^2 \log \tilde{p}(\boldsymbol{\xi}; \boldsymbol{\theta})}{\partial \xi_j^2}$$

Proof (general idea)

- Use Euclidean distance and expand the objective function J_{sm}

$$
\begin{aligned}
J_{\mathrm{sm}}(\boldsymbol{\theta}) &= \frac{1}{2}\mathbb{E}_* \|\boldsymbol{\psi}(\mathbf{x};\boldsymbol{\theta}) - \boldsymbol{\psi}_*(\mathbf{x})\|^2 \\
&= \frac{1}{2}\mathbb{E}_* \|\boldsymbol{\psi}(\mathbf{x};\boldsymbol{\theta})\|^2 - \mathbb{E}_* \left[\boldsymbol{\psi}(\mathbf{x};\boldsymbol{\theta})^\top \boldsymbol{\psi}_*(\mathbf{x})\right] + \frac{1}{2}\mathbb{E}_* \|\boldsymbol{\psi}_*(\mathbf{x})\|^2 \\
&= \frac{1}{2}\mathbb{E}_* \|\boldsymbol{\psi}(\mathbf{x};\boldsymbol{\theta})\|^2 - \sum_{j=1}^{d} \mathbb{E}_* \left[\psi_j(\mathbf{x};\boldsymbol{\theta})\psi_{*,j}(\mathbf{x})\right] + \text{const}
\end{aligned}
$$

- First term does not depend on $\boldsymbol{\psi}_*$. The ψ_j and $\psi_{*,j}$ are the j-th elements of the vectors $\boldsymbol{\psi}$ and $\boldsymbol{\psi}_*$, respectively. Constant does not depend on $\boldsymbol{\theta}$.
- The trick is to use integration by parts for the second term to get an objective function which does not involve $\boldsymbol{\psi}_*$.

Proof (not examinable)

$$\begin{aligned}
\mathbb{E}_* \left[\psi_j(\mathbf{x};\boldsymbol{\theta})\psi_{*,j}(\mathbf{x})\right] &= \int_{\boldsymbol{\xi}} p_*(\boldsymbol{\xi})\psi_{*,j}(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})d\boldsymbol{\xi} \\
&= \int_{\boldsymbol{\xi}} p_*(\boldsymbol{\xi})\frac{\partial \log p_*(\boldsymbol{\xi})}{\partial \xi_j}\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})d\boldsymbol{\xi} \\
&= \prod_{k\neq i}\int_{\xi_k}\left(\int_{\xi_j} p_*(\boldsymbol{\xi})\frac{\partial \log p_*(\boldsymbol{\xi})}{\partial \xi_j}\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})d\xi_j\right)d\xi_k \\
&= \prod_{k\neq i}\int_{\xi_k}\left(\int_{\xi_j} \frac{\partial p_*(\boldsymbol{\xi})}{\partial \xi_j}\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})d\xi_j\right)d\xi_k
\end{aligned}$$

Use integration by parts

$$\begin{aligned}
\int_{\xi_j} \frac{\partial p_*(\boldsymbol{\xi})}{\partial \xi_j}\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})d\xi_j &= \left[p_*(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})\right]_{a_j}^{b_j} - \int_{\xi_j} p_*(\boldsymbol{\xi})\frac{\partial \psi_j(\boldsymbol{\xi};\boldsymbol{\theta})}{\partial \xi_j}d\xi_j \\
&= -\int_{\xi_j} p_*(\boldsymbol{\xi})\frac{\partial \psi_j(\boldsymbol{\xi};\boldsymbol{\theta})}{\partial \xi_j}d\xi_j,
\end{aligned}$$

where the a_j and b_j specify the boundaries of the data pdf p_* along dimension j and where we assume that $\left[p_*(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})\right]_{a_j}^{b_j} = 0$.

Proof (not examinable)

If $[p_*(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})]_{a_j}^{b_j} = 0$

$$
\begin{aligned}
\mathbb{E}_*\left[\psi_j(\mathbf{x};\boldsymbol{\theta})\psi_{*,j}(\mathbf{x})\right] &= -\prod_{k\neq i}\int_{\xi_k}\left(\int_{\xi_j} p_*(\boldsymbol{\xi})\frac{\partial\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})}{\partial\xi_j}d\xi_j\right)d\xi_k \\
&= -\int_{\boldsymbol{\xi}} p_*(\boldsymbol{\xi})\frac{\partial\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})}{\partial\xi_j}d\boldsymbol{\xi} \\
&= -\mathbb{E}_*\left[\partial_j\psi_j(\mathbf{x};\boldsymbol{\theta})\right]
\end{aligned}
$$

so that

$$
\begin{aligned}
J_{\mathrm{sm}}(\boldsymbol{\theta}) &= \frac{1}{2}\mathbb{E}_*\|\boldsymbol{\psi}(\mathbf{x};\boldsymbol{\theta})\|^2 - \sum_{j=1}^{d} -\mathbb{E}_*\left[\partial_j\psi_j(\mathbf{x};\boldsymbol{\theta})\right] + \text{const} \\
&= \mathbb{E}_*\sum_{j=1}^{d}\left[\partial_j\psi_j(\mathbf{x};\boldsymbol{\theta}) + \frac{1}{2}\psi_j^2(\mathbf{x};\boldsymbol{\theta})\right] + \text{const}
\end{aligned}
$$

Replacing the expectation / integration over the data density p_* by a sample average over the observed data gives a computable objective function for score matching.

Final method of score matching

- Given iid data $\mathbf{x}_1, \ldots, \mathbf{x}_n$, the score matching estimate is

$$\hat{\boldsymbol{\theta}} = \operatorname*{argmin}_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

$$J(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{d} \left[\partial_j \psi_j(\mathbf{x}_i; \boldsymbol{\theta}) + \frac{1}{2} \psi_j(\mathbf{x}_i; \boldsymbol{\theta})^2 \right]$$

  ψ_j is the partial derivative of the log unnormalised model $\log \tilde{p}$ with respect to the j-th coordinate (slope) and $\partial_j \psi_j$ its second partial derivative (curvature).

- Parameter estimation with intractable partition functions without approximating the partition function.

Requirements

$$J(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{d}\left[\partial_j\psi_j(\mathbf{x}_i;\boldsymbol{\theta}) + \frac{1}{2}\psi_j(\mathbf{x}_i;\boldsymbol{\theta})^2\right]$$

Requirements:

- technical (from proof): $[p_*(\boldsymbol{\xi})\psi_j(\boldsymbol{\xi};\boldsymbol{\theta})]_{a_j}^{b_j} = 0$, where the a_j and b_j specify the boundaries of the data pdf p_* along dimension j
- smoothness: second derivatives of $\log \tilde{p}(\boldsymbol{\xi};\boldsymbol{\theta})$ with respect to the ξ_j need to exist, and should be smooth with respect to $\boldsymbol{\theta}$ so that $J(\boldsymbol{\theta})$ can be optimised with gradient-based methods.

Simple example

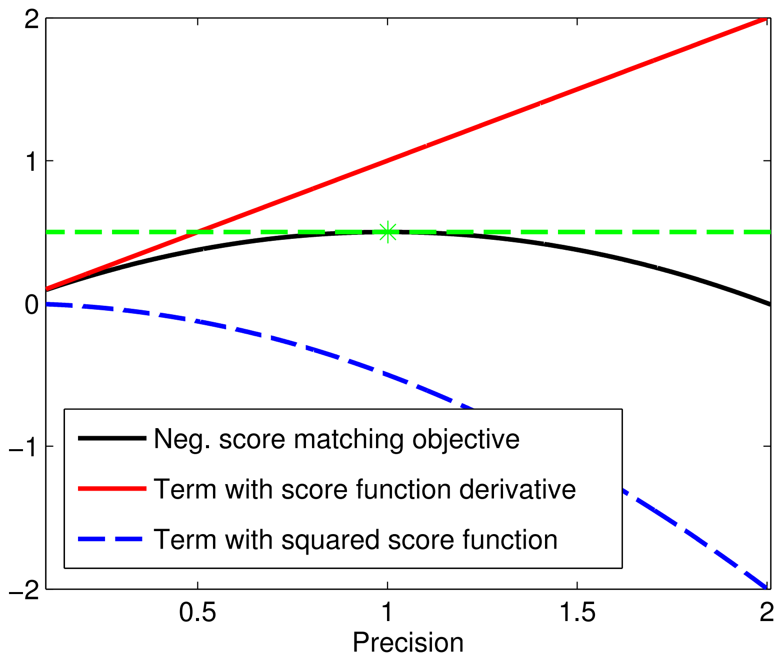
- $\tilde{p}(\xi;\theta) = \exp(-\theta\xi^2/2)$, parameter $\theta > 0$ is the precision.
- The slope and curvature of the log unnormalised model are

$$\psi(\xi;\theta) = \partial_\xi \log \tilde{p}(\xi;\theta) = -\theta\xi, \qquad \partial_\xi \psi(\xi;\theta) = -\theta.$$

- If p_* is Gaussian, $\lim_{\xi\to\pm\infty} p_*(\xi)\psi(\xi;\theta) = 0$ for all θ.
- Score matching objective

$$J(\theta) = {\color{red}-\theta} + {\color{blue}\frac{1}{2}\theta^2 \frac{1}{n}\sum_{i=1}^n x_i^2}$$

$$\Rightarrow \hat{\theta} = \left(\frac{1}{n}\sum_{i=1}^n x_i^2\right)^{-1}$$



- For Gaussians, same as the MLE.

Extensions

- Score matching as presented here only works for $\mathbf{x} \in \mathbb{R}^d$
- There are extensions for discrete and non-negative random variables (not examinable)

  https://www.cs.helsinki.fi/u/ahyvarin/papers/CSDA07.pdf
- Can be shown to be part of a general framework to estimate unnormalised models (not examinable)

  https://michaelgutmann.github.io/assets/papers/Gutmann2011b.pdf
- Overall message: in some situations, other learning criteria than likelihood are preferable.

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