Relating Leverage Scores and Density using Regularized Christoffel Functions

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Outline

1. Leverage scores
2. Main result
3. Technical comments

Outline

Classical statistical leverage scores

- Goal: characterize how points "stick out" and affect the results of a statistical procedure
- Linear regression model:

$$y = X\beta + \epsilon$$

- Ordinary least squares

$$\hat{y} = Hy \quad \text{with} \quad H = X(X^\top X)^{-1}X^\top$$

- Leverage scores:

$$\ell = diag(H)$$

- Property

$$\forall i = 1, \ldots, n \quad \ell_i = \frac{\partial \hat{y}_i}{\partial y_i}$$

λ-ridge leverage scores

- (Kernel) ridge regression

$$\hat{y} = H(\lambda)y \quad \text{with} \quad H(\lambda) = X(X^\top X + n\lambda I_p)^{-1}X^\top = K(K + n\lambda I_n)^{-1}$$

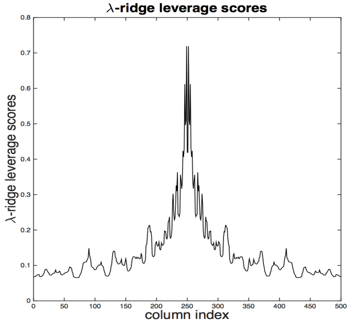
- Leverage scores:

$$\ell(\lambda) = diag(H(\lambda))$$

Use of leverage scores

- Diagnosis tool for linear regression (Hoaglin and Welsch, 1978; Velleman and Welsch, 1981; Chatterjee and Hadi, 1986)
- Matrix sketching and column sampling (Mahoney and Drineas, 2009; Mahoney, 2011; Drineas et al., 2012; Wang and Zhang, 2013)
- Low rank matrix approximation (Clarkson and Woodruff, 2013; Bach, 2013)
- Regression (Alaoui and Mahoney, 2015; Rudi et al., 2015; Ma et al., 2015)
- Random feature learning (Rudi and Rosasco, 2017)
- Quadrature (Bach, 2017).

Open questions: Link between leverage score and density?



"In this experiment, the data points $x_i \in (0, 1)$ have been generated with a distribution symmetric about 1, having a high density on the borders of the interval $(0, 1)$ and a low density on the center of the interval. [...] We can see that there are few data points with high leverage, and those correspond to the region that is underrepresented in the data sample (i.e. the region close to the center of the interval since it is the one that has the lowest density of observations)." (Alaoui and Mahoney, 2015)

Outline

Main result

- For a class of translation-invariant kernels K on $\mathbb{R}^d$
  - E.g., Sobolev space of functions with squared integrable derivatives of order up to $s > d/2$
- For the population λ-ridge leverage score

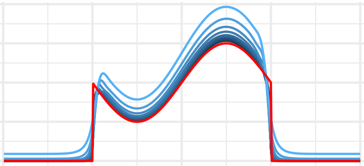
$$\forall z \in \mathbb{R}^d, \quad L_\lambda(z) = \left\langle k(z,\cdot), (\Sigma + \lambda I)^{-1} k(z,\cdot) \right\rangle_{\mathcal{H}_K}$$

- We have, for any $z \in \mathbb{R}^d$ with $p(z) > 0$:

$$L_\lambda(z) \underset{\lambda\to 0,\, \lambda>0}{\sim} L_0 \lambda^{-d/(2s)} p(z)^{d/2s-1}$$

Remarks

$$L_\lambda(z) \underset{\lambda \to 0,\, \lambda > 0}{\sim} L_0 \lambda^{-d/(2s)} p(z)^{d/2s-1}$$



- Explicit relationship between leverage score and density
- Leverage score can be used for density estimation and outlier detection
- May suggest new ways to estimate the leverage score
- Not valid for all kernels (e.g., Gaussian is too smooth)

Outline

Regularized Christoffel function

- Christoffel function, for $l \in \mathbb{N}$:

$$\Lambda_l(z) = \min_{P \in \mathbb{R}_l[X]} \int (P(x))^2 p(x) dx \quad \text{such that} \quad P(z) = 1\,,$$

- NEW: Regularized Christoffel function, for $\lambda > 0$

$$C_\lambda(z) = \inf_{f \in \mathcal{H}} \int_{\mathbb{R}^d} f(x)^2 p(x) dx + \lambda \|f\|_{\mathcal{H}}^2 \quad \text{such that} \quad f(z) = 1\,.$$

- Link with leverage score

$$\forall z \in \mathbb{R}^d\,, \quad C_\lambda(z) = \frac{1}{L_\lambda(z)}$$

Proof sketch

- We study the asymptotics of C_λ
- We show, under some assumptions on the kernel $K(x, y) = q(x - y)$, that:

$$C_\lambda(z) \underset{\lambda \to 0,\, \lambda > 0}{\sim} p(z) D\left(\frac{\lambda}{p(z)}\right),$$

where

$$\begin{aligned} D(\lambda) &:= \min_{f \in \mathcal{H}} \int_{\mathbb{R}^d} f(x)^2 dx + \lambda \|f\|_{\mathcal{H}}^2 \text{ subject to } f(0) = 1 \\ &= \frac{(2\pi)^d}{\int_{\mathbb{R}^d} \frac{\hat{q}(\omega)}{\lambda + \hat{q}(\omega)} d\omega} \end{aligned}$$

Conclusion

- Leverage scores are classical tools in statistics, which gained importance in ML for sketching, sampling, approximating
- We propose a variational formulation of leverage scores, that is an extension of Christoffel functions
- This allows to prove that, under some assumptions on the kernel, leverage scores and proportional to a negative power of the density
- This can suggest new ways to estimate leverage scores, and clarifies why they can be used for density estimation and outlier detection

THANK YOU

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