Supplement of "Detecting non-causal artifacts in multivariate linear regression models"

Dominik Janzing¹ Bernhard Schölkopf²

1. Proofs

1.1. Proof of Lemma 1

We first write Φ as $\Phi(v) = g(Av)Av$, with g(w) := 1/||w||. Let $t \mapsto s(t)$ be some curve on the unit sphere S^{d-1} and $\tilde{s}(t) := \Phi(s(t))$ its image and assume v = s(0) and $\tilde{v} = \tilde{s}(0)$. Then we have

$$\frac{d}{dt}\Phi(s(t)) = \langle \nabla g(As(t)), As'(t) \rangle As(t) +g(As(t))As'(t),$$

with $\nabla g(w) = -w/||w||^3$. Hence we obtain

$$\frac{d}{dt}\Phi(s(t)) \tag{1}$$

$$= \frac{-1}{(As(t),As'(t))As(t) + q(As(t))As'(t))}$$

$$\|As(t)\|^{3} (10(0)) (10(0)) (10(0)) + g(10(0)) (10($$

where we have used
$$\tilde{s}(t) = As(t)/||As(t)||$$
. Note that
the matrix $\mathbf{1} - \tilde{s}(t)\tilde{s}(t)^T$ projects $As'(t)$ onto the space
orthogonal to $\tilde{s}(t)$, that is, the tangent space of the surface
of the sphere at $\tilde{s}(t)$. Further, the matrix

$$g(As(t))\left(\mathbf{1} - \tilde{s}(t)\tilde{s}(t)^T\right)A$$

maps each tangent vector s'(t) at s(t) (for any curve s) to the corresponding tangent vector $\tilde{s}'(t)$ at $\tilde{s}(t)$. It thus describes the Jacobian $D\Phi$ mapping between tangent spaces $T_{s(t)}$ and $T_{\tilde{s}(t)}$ of the sphere at s(t) and $\tilde{s}(t)$, respectively. Let e_1, \ldots, e_{d-1} and $\tilde{e}_1, \ldots, \tilde{e}_{d-1}$ be orthonormal bases of T_v and $T_{\tilde{v}}$, respectively (that is, bases of v^{\perp} and \tilde{v}^{\perp} , respectively). If we set $U_v := (e_1, \ldots, e_{d-1})$ and $U_{\tilde{v}} :=$ $(\tilde{e}_1, \ldots, \tilde{e}_{d-1})$, the matrix representation of the Jacobian $D\Phi$ with respect to these bases reads

$$\widehat{D}\widehat{\Phi}(v) := g(Av)U_{\widetilde{v}}^T A U_v$$

We then have

$$\det D\overline{\Phi}(v) = g(Av)^{d-1} \det(U_{\widetilde{v}}^T A U_v).$$

For later use, we also observe that multiplying the equation $\tilde{v} = Av/\|Av\|$ with A^{-1} and taking the norm on both sides yields

$$1/\|Av\| = \|A^{-1}\tilde{v}\|.$$
(3)

For the probability density we thus obtain

$$p(\tilde{v}) = |\det \widehat{D\Phi}(\Phi^{-1}(\tilde{v}))|^{-1} = (||A^{-1}\tilde{v}||^{d-1} |\det(U_{\tilde{v}}^{T}AU_{v})|)^{-1} = (||A^{-1}\tilde{v}||^{d-1} |\det(\tilde{A})|)^{-1},$$
(4)

with the abbreviation $\tilde{A} := U_{\tilde{v}}^T A U_v$. Let us now define the orthogonal $d \times d$ matrices

$$W_v := (U_v, v)$$
 and $(U_{\tilde{v}}, \tilde{v}).$

Then we define $A' := W_{\tilde{v}}^T A W_v$, which implies $|\det(A')| = |\det(A)|$. A' can be written as

$$A' = \left(\begin{array}{cc} \tilde{A} & 0\\ w & \|Av\| \end{array}\right),$$

where w is some $1 \times (d-1)$ -matrix. Hence we obtain

$$\det(A') = \det(\tilde{A}) \|Av\| = \frac{\det(\tilde{A})}{\|A^{-1}\tilde{v}\|}$$

where we have used also (3). We can thus rewrite (4) as

$$p(\tilde{v}) = \frac{1}{|\det(A)| ||A^{-1}\tilde{v}||^d}.$$

1.2. Proof of Theorem 3

By definition, $p_{\theta'}$ is obtained by applying the map $\sqrt{R_{\theta}}$ to vectors drawn from a rotation invariant distribution with renormalizing it later. Without loss of generality, let all the matrices R_{θ} be diagonal with eigenvalues $f_j(\theta)$ (note that they commute). Let v be generated by drawing each entry v_j from $\mathcal{N}(0, 1)$. We can then compute the entries of \tilde{v} by

$$\tilde{v}_j := \frac{1}{\sum_{i=1}^d f_j(\theta') v_j^2} \sqrt{f_j(\theta')} v_j$$

¹Amazon Development Center, Tübingen, Germany ²Max Planck Institute for Intelligent Systems, Tübingen, Germany. This work has been done at the MPI before DJ joined Amazon. Correspondence to: Dominik Janzing <janzind@amazon.com>.

Proceedings of the 35th International Conference on Machine Learning, Stockholm, Sweden, PMLR 80, 2018. Copyright 2018 by the author(s).

Rewriting (10) in terms of v_j instead of \tilde{v} yields

$$\log p_{\theta}(\tilde{v}) = -\frac{1}{2} \left\{ \log \frac{1}{d} \sum_{j=1}^{d} f_j(\theta') f_j(\theta)^{-1} v_j^2 - \log \frac{1}{d} \sum_{j=1}^{d} f_j(\theta') v_j^2 \right\} + \frac{1}{2} \log \det R_{\theta}$$

Since each v_j^2 is an independent squared standard Gaussian it has expectation 1 and variance 2. Therefore, the random variable

$$\frac{1}{d}\sum_{j=1}^d f_j(\theta')f_j(\theta)^{-1}v_j^2$$

has mean $\tau(R_{\theta}R_{\theta'}^{-1})$ and variance

$$\frac{2}{d^2} \sum_{j=1}^d f_j(\theta')^2 f_j(\theta)^{-2}$$

Due to Chebychev's inequality we have

$$\left|\frac{1}{d}\sum_{j=1}^{d}f_j(\theta')f_j(\theta)^{-1}v_j^2 - \tau(R_{\theta'}R_{\theta}^{-1})\right| \le \delta_j$$

with probability $1 - \frac{2}{d^2} \sum_{j=1}^d f_j(\theta')^2 f_j(\theta)^{-2}/\delta^2 = 1 - \frac{2}{d}\tau(R_{\theta'}^2 R_{\theta}^{-2})/\delta^2$. Likewise,

$$\left|\frac{1}{d}\sum_{j=1}^{d}f_{j}(\theta')v_{j}^{2}-\tau(R_{\theta'})\right|\leq\delta,$$

with probability $1 - \frac{2}{d}\tau(R_{\theta'}^2)/\delta^2$. Since $|\log(x + \rho) - \log x| \le 2\rho/x$ for sufficiently small ρ , we can ensure that

$$\left|\log\frac{1}{d}\sum_{j=1}^{d}f_{j}(\theta')f_{j}(\theta)^{-1}v_{j}^{2}-\log\tau(R_{\theta'}R_{\theta}^{-1})\right|\leq\epsilon,\quad(5)$$

by choosing $\delta \leq \epsilon/(2\tau(R_{\theta'}R_{\theta}^{-1})).$ Likewise, we can achieve that

$$\left|\log\frac{1}{d}\sum_{j=1}^{d}f_{j}(\theta')v_{j}^{2} - \log\tau(R_{\theta'})\right| \leq \epsilon, \qquad (6)$$

if $\delta \leq \epsilon/(2\tau(R_{\theta'}))$. Thus, both inequalities (5) and (6) together hold with probability at least

$$1 - \frac{8}{d\epsilon^2} \left[\tau(R_{\theta'}^2 R_{\theta}^{-2}) \tau(R_{\theta'} R_{\theta}^{-1})^2 + \tau(R_{\theta'}^2) \tau(R_{\theta'})^2 \right].$$