

Stein method for quadratic forms

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Theorem 1. Let ζ_1, \dots, ζ_d be iid random variables with mean 0 and variance 1, and assume $\mu_k := \mathbb{E}(\zeta_1^k)$ is finite for $k \leq 8$. Let $\boldsymbol{\zeta} = (\zeta_1, \dots, \zeta_d)^\top \in \mathbb{R}^d$. For $k = 1, \dots, K$, let $\mathbf{Q}_k = (q_{ij}^{(k)})$ be a $d \times d$ symmetric matrix and let $\check{\mathbf{Q}}_k = \text{diag}(q_{11}^{(k)}, \dots, q_{dd}^{(k)})$, $\hat{\mathbf{Q}}_k = \mathbf{I}_d - \check{\mathbf{Q}}_k$. Define $\hat{w}_k = \boldsymbol{\zeta}^\top \hat{\mathbf{Q}}_k \boldsymbol{\zeta}$, $\check{w}_k = \boldsymbol{\zeta}^\top \check{\mathbf{Q}}_k \boldsymbol{\zeta} - \text{tr}(\mathbf{Q}_k)$, and

$$W = \begin{pmatrix} \hat{w}_1 \\ \check{w}_1 \\ \vdots \\ \hat{w}_K \\ \check{w}_K \end{pmatrix} = \begin{pmatrix} \boldsymbol{\zeta}^\top \hat{\mathbf{Q}}_1 \boldsymbol{\zeta} \\ \boldsymbol{\zeta}^\top \check{\mathbf{Q}}_1 \boldsymbol{\zeta} - \text{tr}(\mathbf{Q}_1) \\ \vdots \\ \boldsymbol{\zeta}^\top \hat{\mathbf{Q}}_K \boldsymbol{\zeta} \\ \boldsymbol{\zeta}^\top \check{\mathbf{Q}}_K \boldsymbol{\zeta} - \text{tr}(\mathbf{Q}_K) \end{pmatrix} \in \mathbb{R}^{2K}.$$

Finally, let $Z \sim \mathcal{N}_{2K}(0, \mathbf{I}_{2K})$ and $\mathbf{V} = \text{Cov}(W)$. There is an absolute constant $0 < C < \infty$ such that

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Proof. Let $f : \mathbb{R}^{2K} \rightarrow \mathbb{R}$ be a four-times differentiable function. From xxx, there is a 4 – times differentiable function $g : \mathbb{R}^{2K} \rightarrow \mathbb{R}$ satisfying the Stein identity

$$\mathbb{E}[f(W)] - \mathbb{E}[f(\mathbf{V}^{1/2}W)] = \mathbb{E}[\nabla^\top \mathbf{V} \nabla g(W) - W^\top \nabla g(W)]$$

and

$$\left| \frac{\partial^k g(\mathbf{x})}{\prod_{j=1}^k \partial x_{i_j}} \right| \leq \frac{1}{k} \left| \frac{\partial^k f(\mathbf{x})}{\prod_{j=1}^k \partial x_{i_j}} \right| \quad \text{for all } \mathbf{x} = (x_1, \dots, x_{2K})^\top \in \mathbb{R}^{2K}, k = 1, 2, 3, \text{ and } i_j \in \{1, \dots, 2K\}.$$

To prove the theorem, we bound

$$S = \mathbb{E}[\nabla^\top \mathbf{V} \nabla g(W) - W^\top \nabla g(W)].$$

Next, we use exchangeability. Let $\boldsymbol{\zeta}' = (\zeta'_1, \dots, \zeta'_d)^\top$ be an independent copy of $\boldsymbol{\zeta}$, and let $\underline{i} \in \{1, \dots, d\}$ be an independent and uniformly distributed random index. Define the vector

$W' \in \mathbb{R}^{2K}$ exactly as we defined W , except that $\zeta_{\underline{i}}$ is replaced with $\zeta'_{\underline{i}}$ throughout. More precisely, let $e_i \in \mathbb{R}^d$ be the i th standard basis vector in \mathcal{R}^d and define

$$\begin{aligned}\hat{w}'_k &= (\zeta + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}})^\top \hat{\mathbf{Q}}_k (\zeta + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}}) \\ &= \hat{w}_k + 2(\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}}^\top \hat{\mathbf{Q}}_k \zeta,\end{aligned}$$

$$\begin{aligned}\check{w}'_k &= (\zeta + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}})^\top \check{\mathbf{Q}}_k (\zeta + (\zeta'_{\underline{i}} - \zeta_{\underline{i}})e_{\underline{i}}) - \text{tr}(\mathbf{Q}_k) \\ &= \check{w}_k + e_{\underline{i}}^\top \check{\mathbf{Q}}_k e_{\underline{i}} ((\zeta'_{\underline{i}})^2 - \zeta_{\underline{i}}^2),\end{aligned}$$

for $k = 1, \dots, K$. Then $W' = (\hat{w}'_1, \check{w}'_1, \dots, \hat{w}'_K, \check{w}'_K)^\top \in \mathbb{R}^{2K}$. Its straightforward to verify that

$$\mathbb{E}(\hat{w}'_k - \hat{w}_k | \zeta) = -\frac{2}{d}\hat{w}_k, \quad \mathbb{E}(\check{w}'_k - \check{w}_k | \zeta) = -\frac{1}{d}\check{w}_k.$$

Then

$$\mathbb{E}(W' - W | \zeta) = -\Lambda_K W,$$

where

$$\Lambda_1 = \begin{pmatrix} \frac{2}{d} & 0 \\ 0 & \frac{1}{d} \end{pmatrix}, \quad \Lambda_K = \begin{pmatrix} \Lambda_1 & 0 & \cdots & 0 \\ 0 & \Lambda_1 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \Lambda_1 \end{pmatrix} \in \mathbb{R}^{2K \times 2K}.$$

By exchangeability, we have

$$\begin{aligned}0 &= \frac{1}{2} \mathbb{E}[(W' - W)^\top \Lambda_K^{-\top} (\nabla g(W') + \nabla g(W))] \\ &= \mathbb{E}[(W' - W)^\top \Lambda_K^{-\top} \nabla g(W)] + \frac{1}{2} \mathbb{E}[(W' - W)^\top \Lambda_K^{-\top} (\nabla g(W') - \nabla g(W))] \\ &= -\mathbb{E}[W^\top \nabla g(W)] + \frac{1}{2} \mathbb{E}[(W' - W)^\top \Lambda_K^{-\top} (\nabla g(W') - \nabla g(W))].\end{aligned}$$

That is,

$$\mathbb{E}[W^\top \nabla g(W)] = \frac{1}{2} \mathbb{E}[(W' - W)^\top \Lambda_K^{-\top} (\nabla g(W') - \nabla g(W))].$$

Apply Taylor's theorem,

$$\begin{aligned}& W^\top \nabla g(W) \\ &= \frac{1}{2} \sum_{i,j=1}^{2K} \Lambda_{K,ii}^{-1} D^{ij} g(W) (w'_i - w_i)(w'_j - w_j) + \frac{1}{4} \sum_{i,j,k=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijk} g(W) (w'_i - w_i)(w'_j - w_j)(w'_k - w_k) \\ &\quad + \frac{1}{12} \sum_{i,j,k,l=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijkl} g(t^*(W' - W) + W) (w'_i - w_i)(w'_j - w_j)(w'_k - w_k)(w'_l - w_l) \\ &= \frac{1}{2} \text{tr}[(W' - W)(W' - W)^\top \Lambda_K^{-\top} \nabla^2 g(W)] + \frac{1}{4} \sum_{i,j,k=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijk} g(W) (w'_i - w_i)(w'_j - w_j)(w'_k - w_k) \\ &\quad + \frac{1}{12} \sum_{i,j,k,l=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijkl} g(t^*(W' - W) + W) (w'_i - w_i)(w'_j - w_j)(w'_k - w_k)(w'_l - w_l),\end{aligned} \tag{1}$$

where $t^* \in [0, 1]$. Also by exchangeability,

$$\mathbb{E}[(W' - W)(W' - W)^\top] = 2 \mathbb{E}[W(W - W')^\top] = 2 \mathbb{E}[WW^\top \Lambda_K^\top] = 2\mathbf{V}\Lambda_K^\top.$$

It follows that

$$\mathbb{E}[\nabla^\top \mathbf{V} \nabla g(W)] = \mathbb{E} \operatorname{tr}[\mathbf{V} \nabla^2 g(W)] = \frac{1}{2} \mathbb{E} \operatorname{tr}[\mathbb{E}[(W' - W)(W' - W)^\top] \Lambda_K^{-\top} \nabla^2 g(W)]$$

Thus,

$$\begin{aligned} S &= \mathbb{E}[\nabla^\top \mathbf{V} \nabla g(W) - W^\top \nabla g(W)] \\ &= \frac{1}{2} \mathbb{E} \operatorname{tr}[\mathbb{E}[(W' - W)(W' - W)^\top] \Lambda_K^{-\top} \nabla^2 g(W)] - \frac{1}{2} \mathbb{E} \operatorname{tr}[(W' - W)(W' - W)^\top \Lambda_K^{-\top} \nabla^2 g(W)] \\ &\quad - \frac{1}{4} \mathbb{E} \sum_{i,j,k=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijk} g(W) (w'_i - w_i)(w'_j - w_j)(w'_k - w_k) \\ &\quad - \frac{1}{12} \mathbb{E} \sum_{i,j,k,l=1}^{2K} \Lambda_{K,ii}^{-1} D^{ijkl} g(t^*(W' - W) + W) (w'_i - w_i)(w'_j - w_j)(w'_k - w_k)(w'_l - w_l). \end{aligned}$$

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