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Stein's Method in Stochastic Geometry, Statistical Learning, and Optimisation

Organized by
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Abstract. Stein's method, a powerful tool rooted in probability and stochastic analysis, has recently showcased its efficacy in addressing diverse challenges encountered in deep learning, optimisation, sampling, and causal inference. The primary focus of the workshop is to strengthen the probabilistic and analytic foundations of Stein's method, while simultaneously exploring novel avenues for its application. Bringing together researchers from the analysis, probability, statistics, and machine learning communities, who share a common interest in Stein's method, the workshop aims to facilitate idea exchange, tackle open problems, and foster collaborations to advance the forefront of knowledge in these fields. Of particular importance is the emphasis placed on the intersection of these disciplines, where Stein's method plays a pivotal role.

Mathematics Subject Classification (2020): 60D05, 62E17, 65C05, 65K99, 68P27, 68T99.

Introduction by the Organizers

The half workshop *Stein's Method in Stochastic Geometry, Statistical Learning, and Optimisation*, organized by Krishnakumar Balasubramanian (Davis), Murat A. Erdogdu (Toronto), Larry Goldstein (Los Angeles), and Gesine Reinert (Oxford), attracted over 20 researchers worldwide with diverse backgrounds and at various career stages. After a small number of introductory talks, participants were encouraged to suggest and form working groups on open problems. These groups periodically reported back to the workshop at large, sharing progress and receiving feedback on possible approaches. At the close of the meeting, participants arranged modes of continued collaboration to extend their work beyond the week at Oberwolfach.

Scope and Themes

The workshop explored the rapidly developing interface between Stein's method and contemporary problems in stochastic geometry, statistics, and data science. The central theme was to advance both the analytic foundations of Stein's method and its application to pressing questions in diverse areas such as privacy, learning theory, dependence structures, geometric probability, and approximation theory. A distinctive feature of the workshop was the breadth of disciplines represented – ranging from classical probability to current applications in data science – underscoring the unifying role Stein's method can play across these domains.

The working group format proved especially effective in fostering concentrated discussions and stimulating new directions of research.

Working Groups and Results

Several working groups formed organically over the course of the week:

- **Data Privacy.** One group investigated how Stein's method may provide utility guarantees for differentially private mechanisms. Differential privacy offers quantitative bounds on the risk of recovering individual items from a database after a sanitizing mechanism has been applied, with utility typically measured via distances between the distributions of the original and sanitized data. For explicit mechanisms such as the exponential, and under a statistical model for the underlying database, Stein operators can be employed to analyze the discrepancy between the true and sanitized distributions. The discussions during the week clarified the potential of this approach and identified several concrete directions for further research.
- **Extensions of Slepian's Inequality.** Considerable progress was made in extending Slepian's classical Gaussian comparison inequality to broader contexts. Building on the interpolation method, the group demonstrated that an analogous argument can be carried out along trajectories generated by optimal transport between distributions. This insight opens the door to comparison principles beyond the Gaussian setting, with potential implications for dependent structures in high-dimensional statistics and learning theory.
- **Extreme Value Approximations for Geometric Functionals.** This group examined limiting laws for functionals of Poisson processes, focusing on extreme value behavior. By analyzing a sandbox model with significant dependence, the group established what appear to be optimal error rates in approximating the Gumbel distributional limit. Their approach combined a direct analysis of the Stein equation for the Gumbel, though coupling techniques based on fixed-point characterizations were also considered. The methods developed should generalizable to more complex

situations, such as the maximum nearest neighbor distances of points of Poisson process, having applications in high dimensional statistics.

- **Dickman Approximation.** Another group extended the reach of Dickman-type limits by identifying close couplings for the classical case of sums of weighted indicators that converge to the Dickman distribution. Their construction enabled sharper Wasserstein-1 distance bounds, improving upon existing results and suggesting generalizations to broader classes of combinatorial structures, such as networks that grow over time, such as those on the web.
- **Additional Explorations.** Other participants pursued potential characterizations of the uniform distribution on high-dimensional spheres, connecting Stein's method to further geometric techniques. These efforts underscored the versatility of the method and its adaptability to novel probabilistic settings.

Concluding Remarks

The workshop was marked not only by technical achievements but also by a lively spirit of collaboration. The Oberwolfach environment, with its distinctive blend of intellectual intensity and informal camaraderie, was central to the success of the meeting. Participants took full advantage of the bicycles, running paths, and the music room, and many commented on how these activities enriched the scientific exchanges. The parallel workshop taking place during the same week provided further opportunities for cross-fertilization of ideas, with several joint discussions revealing unexpected common ground.

The organizers are especially grateful to the Oberwolfach staff for their outstanding support, which ensured that all aspects of the workshop ran smoothly. The atmosphere of openness, curiosity, and collegiality fostered during the week has already led to concrete collaborations, and we are confident that the Overleaf projects created by these groups before the end of the meeting will guarantee the continued interactions of these groups in the future.

Workshop: Stein's Method in Stochastic Geometry, Statistical Learning, and Optimisation

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Abstracts

Stein's Method and Stochastic Geometry

Joseph Yukich

This talk surveys some of the interactions between stochastic geometry and Stein's method of normal approximation. The talk reviews the following topics: (i) dependency graphs and their utility in establishing quantitative CLTs (ii) martingale difference methods (iii) weakly stabilizing Poisson functionals (iv) Malliavin-Stein methods applied to Poisson functionals (v) stabilizing score functions and the normal approximation of sums of stabilizing scores in the univariate and multivariate CLT.

Random Networks: Questions, Models, Approaches. A brief Overview.

Gesine Reinert

In this talk, first real-life examples of networks are introduced to motivate the small-world phenomenon. These examples include Padgett's Florentine family marriage network, Zachary's karate club network, a protein-protein interaction network for yeast, a trade network, a political blog network, and an internet network. In many real-world network, high local clustering jointly occurring with with relatively short shortest path lengths is observed.

To explain this phenomenon, a range of models are surveyed, such as Bernoulli random graphs, Watts-Strogatz small world networks, Barabási-Albert models, configuration models, the Chung-Lu model, geometric random graph models, exponential random graph models, and duplication-divergence models. Here, new developments regarding duplication-divergence models with edge deletion are highlighted.

Then several approaches for assessing the probabilistic behaviour of local and global structures in random networks are discussed: Stein's method for subgraph counts, percolation for connectedness, branching process approximations for shortest path lengths, and localisation as well as stabilisation methods for local spatial statistics. A general question arises: When can we approximate an involved network model by a simpler network model? This is the kind of question which can often be addressed using Stein's method. In this talk, for comparing random network models using Stein's method, first the generator approach, using Glauber dynamics, is given. Results for approximating exponential random graph models by Bernoulli random graphs are detailed. Then new results on adapting the Stein density approach to networks are provided.

The talk touches on some success stories of network analysis: detecting unusual structures in co-memberships of board of directors in large companies, identifying essential proteins based on their position in a protein-protein interaction network (which is relevant in network pharmacology), identifying anomalies in networks of financial transactions, and nowcasting GDP from trade flow network data The talk concludes with an outlook, including issues in time series of networks, hypergraphs, and spatio-temporal networks.

Learning Quadratic Neural Networks in High-dimensions

Murat A. Erdogdu

We study the optimization and sample complexity of gradient based training of a two-layer student neural network with quadratic activation function in the high-dimensional regime, where the input is Gaussian and the response is generated from a two-layer teacher network with quadratic activation, and the power law decay on the second layer coefficients. We provide a sharp analysis of the SGD dynamics in the feature learning regime, and derive scaling laws for the prediction risk that highlight the power-law dependences on the optimization time, sample size, and model width.

This result demonstrates the effect of data distribution on neural scaling laws, and reconciles recent theoretical studies with frontier AI practice. The performance of modern AI models critically depends on how computational resources are allocated – particularly between model size and training duration. Empirical studies consistently demonstrate a power-law relationship between compute budget and performance: the optimal model size scales as n^{ξ} while the loss decreases as $n^{-\eta}$, where n is the total computational budget. These scaling laws offer valuable guidance for efficient model design and resource allocation, and have become central to training large-scale neural networks.

Specifically, our setting allows for an extensive number of signals to be learned from data, as one would expect to see in practice, and we proved that neural networks can efficiently recover those signals. Our crucial contribution is that we present a sharp analysis of the SGD dynamics in the feature learning regime, and derive scaling laws for the prediction risk that highlight the power-law dependencies on the optimization time, sample size, and model width. This analysis combines a precise characterization of the associated matrix Riccati differential equation with novel matrix monotonicity arguments to establish convergence guarantees for the infinite-dimensional effective dynamics. The importance of this work is two-fold: (i) it is the first work to demonstrate scaling laws in the feature learning regime (ii) it reconciles the practical neural scaling laws behaviour with the recent single-index/SGD analysis developed by Ben Arous et al.

Stein's method for spatial random graphs

Leoni Wirth

Spatial random graphs provide an important framework for the analysis of relations and interactions in networks. In particular, the random geometric graph has been intensively studied and applied in various frameworks like network modeling or percolation theory.

In this talk we focus on approximation results for a generalization of the random geometric graph that consists of vertices given by a Gibbs process and (cond.) independent edges generated from a connection function. Using Stein's method, we compare this graph model with general spatial random graphs with respect to general integral probability metrics, providing concrete rates in the case of a suitable Wasserstein metric. We then present an application of our results to the soft Boolean model. Finally, we describe how associated kernel Stein discrepancies can be used for goodness-of-fit testing in the framework of point processes and, as future work, spatial random graphs.

Stein's method for the Dickman distribution

Matthias Schulte
(joint work with Chinmoy Bhattacharjee)

The aim of this research is to derive bounds for the Kolmogorov distance between certain weighted sums of independent random variables and the so-called Dickman distribution by Stein's method. The details can be found in the paper [4].

The Dickman function $\varrho : [0,\infty) \to [0,\infty)$ is the solution of the differential delay equation

$$x\varrho'(x) + \varrho(x-1) = 0, \quad x \in (1,\infty),$$

with the initial condition $\varrho(x) = 1$ for $x \in [0,1]$ and appeared first in the work by Dickman on smooth numbers [5]. For independent random variables $(U_k)_{k\in\mathbb{N}}$ uniformly distributed on $[0,1]$ the random variable

$$D = \sum_{j=1}^{\infty} \prod_{k=1}^{j} U_k = U_1 + U_1U_2 + U_1U_2U_3 + \dots$$

has, surprisingly, a constant times the Dickman function as density. Its distribution is called the standard Dickman distribution and satisfies the distributional fixed point equation

$$D \stackrel{d}{=} U(1+D),$$

where U is uniformly distributed on $[0,1]$ and independent of D. More generally, one says that a random variable D_θ follows a Dickman distribution with parameter $\theta \in (0,\infty)$ if

$$D_\theta \stackrel{d}{=} U^{1/\theta}(1+D_\theta)$$

with U uniformly distributed on $[0,1]$ and independent of D_θ. For further details on the Dickman distribution we refer to the survey [10].

The Dickman distribution arises as limiting distribution in different contexts such as logarithmic combinatorial structures [2], the running time of the Quickselect algorithm [7, 8], or edge-length functionals of the minimal directed spanning tree [11]. A typical situation is that, for a fixed $\theta \in (0,\infty)$ and a sequence of independent Bernoulli distributed random variables $(B_k)_{k\geq\lceil\theta\rceil}$ such that

$\mathbf{P}(B_k = 1) = \frac{\theta}{k}$ for $k \geq \lceil \theta \rceil$,

$$\frac{1}{n} \sum_{k=\lceil \theta \rceil}^{n} k B_k \xrightarrow{d} D_\theta \quad \text{as} \quad n \to \infty.$$

In such cases, we are interested in rates of convergence for the Kolmogorov distance. The latter is given by

$$d_K(Y, Z) = \sup_{a \in [0,\infty)} |\mathbf{P}(Y \leq a) - \mathbf{P}(Z \leq a)|$$

for two non-negative random variables Y and Z. One of our main results is as follows:

Theorem 1 (Theorem 1.1 in [4]). *For $\theta > 0$, $\beta \in \mathbb{R}$ and $n, l \in \mathbb{N}$ with $n \geq l \geq \theta - \beta$, let $W_n = \frac{1}{n} \sum_{k=l}^{n} k B_k$ with independent Bernoulli distributed random variables $(B_k)_{k \geq l}$ such that $\mathbf{P}(B_k = 1) = \frac{\theta}{k+\beta}$ for $k \geq l$. Then, there exists a constant $C \in (0, \infty)$ depending only on θ and β such that*

$$d_K(W_n, D_\theta) \leq \begin{cases} \frac{C(l + |\beta| \log(n/l))}{n}, & \theta \geq 1, \\ \frac{C l^\theta}{n^\theta}, & \theta \in (0, 1). \end{cases}$$

For $\theta \geq 1$ the rate of convergence in Theorem 1 slows down for $\beta \neq 0$ by an additional logarithmic factor. By deriving lower bounds for the Kolmogorov distance, one can show that the bound in Theorem 1 is of optimal order in n.

A result analogous to Theorem 1 remains valid if the underlying independent Bernoulli distributed random variables are replaced by independent Poisson distributed random variables with the same parameters. For a similar bound in the Poisson case we refer to [2, Theorem 11.12]. As its proof relies on properties of the Poisson distribution, it is unclear if the approach of [2], which also employs Stein's method, can be used for weighted sums of Bernoulli distributed random variables. The works [1, 3, 6] on Dickman approximation via Stein's method do not consider the Kolmogorov distance but distances based on smooth test functions.

The idea of Stein's method for the Dickman distribution (see [2, 6]) is to consider the Stein equation

$$\frac{x}{\theta} f'(x) + f(x) - f(x+1) = h(x) - \mathbf{E}[h(D_\theta)], \quad x \in [0, \infty),$$

for a given test function $h : [0, \infty) \to \mathbb{R}$. For the Kolmogorov distance, one has to study the case $h = \mathbf{1}_{[0,a]}$ with $a \in (0, \infty)$. We show that there exists a solution f_a whose derivative has certain boundedness and monotonicity properties. This allows us to control

$$\left| \mathbf{E}\left[\frac{W_n}{\theta} f_a'(W_n) + f_a(W_n) - f_a(W_n + 1) \right] \right|.$$

Since our upper bound on that quantity becomes large for small a, we employ a lemma that, for $a_0 \in (0, \infty)$,

$$d_K(W_n, D_\theta) \leq \sup_{a \geq a_0} |\mathbf{P}(W_n \leq a) - \mathbf{P}(D_\theta \leq a)| + R_{\theta, a_0}$$

with an error term R_{θ,a_0} depending on θ and a_0, and choose a_0 as a function of n. This proof is for the even more general situation that W_n is a weighted sum of certain independent random variables that are themselves sums of independent Bernoulli distributed random variables.

Some arguments of the proof are employed in [9], where Dickman approximation is used to study the content of m-smooth numbers with respect to certain probability measures.

The minimal directed spanning tree is a spatial random graph whose vertices are the points of a homogeneous Poisson process η_s with intensity $s > 0$ on $[0,1]^2$ and the origin. Each point of η_s is connected by an edge to the closest coordinate-wise smaller vertex (i.e., its nearest neighbour in the south-west). In [11], it is shown that sums of powers of the lengths of edges incident to the origin converge in distribution to a Dickman distribution, i.e.,

$$\sum_{x\in\eta_s} \mathbf{1}\{0 \leftrightarrow x\}\|x\|^\tau \xrightarrow{d} D_{2/\tau} \quad \text{as} \quad s\to\infty$$

for $\tau > 0$, where $0 \leftrightarrow x$ indicates an edge between 0 and x. These edge-length functionals are not weighted sums of independent random variables. In an ongoing work, we aim to derive rates of convergence for this limit theorem.

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Kernel Stein discrepancy (KSD) for comparing and testing distributions

Wenkai Xu

Stein's method provides a strong ground to compare and bound distributions, e.g. for normal distributions or Poisson distributions. By considering measures in the form of Integral Probability Metric (IPM), distribution bounds are provided via Wasserstein distance, total variation distance, etc. However, the supreme norm over specified test function class may not be easily achieved/computed in the IPM. In this talk, we introduce the Reproducing Kernel Hilbert Space (RKHS) as the test function class to compute the Stein discrepancy in closed-form. The Stein operator used also enable the KSD to address unnormalized models where computing of partition function is prohibitive. Moreover, we introduce KSD-based testing procedure beyond Euclidean space, including Riemannian manifold, simplex, and others.

Stein's method for Fréchet approximation

Yvik Swan

We develop a new approach to quantitative approximation of extreme value laws in the Fréchet domain using Stein's method. Building on the generator comparison framework, we derive explicit, tractable bounds on the Kolmogorov, total variation, and Wasserstein distances between the normalized maximum of i.i.d. samples and the Fréchet limit. Our bounds are expressed in terms of a Stein-type discrepancy measuring the deviation from regular variation, and allow for sharp convergence rates across a wide range of classical distributions. Applications include detailed analyses of Student-t, Burr, Cauchy, and Pareto maxima.

Normal Approximation for Sums of Scores

Tara Trauthwein
(joint work with Joseph Yukich)

We study functions of Poisson point processes which can be expressed as sums of scores, i.e. $F = \sum_{x \in P} \xi(x, P)$. Under weak conditions on the functions ξ, we can show quantitative CLTs with good speeds of convergence. The score functions ξ need to 'localize' with high probability, they need to be close in law to the same function evaluated on a finite but large neighborhood. This is a significantly weaker requirement than what is known as 'stabilization'. Our proofs are based on the Malliavin-Stein method. In particular, we establish a new second-order Poincaré inequality for the normal approximation of general Poisson functionals under 4th moment assumptions, a result which extends work from (Last, Peccati, Schulte 2016) and (Trauthwein 2025). The new bound removes spurious terms which were present in previous works and adds marks. Applications include local U-statistics in metric spaces, stabilization in hyperbolic space, random sequential adsorption, Spin systems and more. This talk is based on joint work with Joseph Yukich.

Normal approximation for exponential random graphs

Xiao Fang

(joint work with Song-Hao Liu, Qi-Man Shao, Yi-Kun Zhao)

We use Stein's method to prove the central limit theorem (CLT) for the total number of edges in exponential random graph models. As a result of our proof, we also derive a convergence rate for the CLT, an explicit formula for the asymptotic variance, and the CLT for general subgraph counts. This is joint work with Song-Hao Liu, Qi-Man Shao, and Yi-Kun Zhao.

Efficient finite sample guarantees by Gaussian approximation

Morgane Austern

Concentration inequalities for the sample mean, such as those by Bernstein and Hoeffding, are valid for any sample size but often yield overly conservative confidence intervals. In contrast, the central limit theorem (CLT) provides asymptotically optimal intervals, but these lack validity for finite samples. To bridge this gap, we develop new computable concentration inequalities with asymptotically optimal size, finite-sample validity, and sub-Gaussian decay. These results enable efficient construction of confidence intervals with correct coverage for any sample size, as well as empirical Berry-Esseen bounds that require no prior knowledge of the population variance. We achieve these bounds via tight control of non-uniform Kolmogorov and Wasserstein distances to a Gaussian using zero-bias couplings and Stein's method of exchangeable pairs. Complementing these advances, we propose a computable version of the Komlós–Major–Tusnády (KMT) inequality for partial sums of bounded i.i.d. random variables, addressing its reliance on unknown constants. By introducing an additional logarithmic factor, our version depends only on the variables' range and standard deviation, and we further derive an empirical variant that achieves nominal coverage without prior knowledge of the standard deviation. We illustrate the utility of these bounds through applications to online change point detection and first hitting time probabilities, highlighting their practicality in real-world scenarios.

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