Local and Global Methods to Identify Local and Global Structure in Data Science

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Start with the conclusions

Practice:

- Some problems are "global":
 - total click-through rate; total number of stars; human population genetics
- Some problems are "local":
 - meaningful communities; quasars that identify new physics; personalized medicine

Theory:

- Most objectives are global:
 - global partition, global eigenvetor, global minimum
- Some objectives are local:
 - find good cluster near a seed set
- Most algorithms are local:
 - take one step of gradient descent
 - but theory then makes a statement about global objective
 - but practice then deviates from theory and applies it locally

Question: How to go forward?



Randomized Numerical Linear Algebra

Structure in Social and Other Informatics Graphs

Why Deep Learning Works

Matrix computations

- Eigendecompositions, QR, SVD, least-squares, etc.
- Traditional algorithms:
 - compute "exact" answers to, say, 10 digits as a black box
 - assume the matrix is in RAM and minimize flops
- But they are NOT well-suited for:
 - with missing or noisy entries
 - problems that are very large
 - distributed or parallel computation
 - when communication is a bottleneck
 - when the data must be accessed via "passes"

The general idea ...

- Randomly sample columns/rows/entries of the matrix, with carefully-constructed *importance sampling probabilities*, to form a randomized sketch
- Preprocess the matrix with random projections, to form a randomized sketch by sampling columns/rows uniformly
- Use the sketch to compute an approximate solution to the original problem w.h.p.
- Resulting sketches are "similar" to the original matrix in terms of singular value and singular vector structure, e.g., w.h.p. are bounded distance from the original matrix

History of Randomized Matrix Algs

Theoretical origins

- theoretical computer science, convex analysis, etc.
- Johnson-Lindenstrauss
- Additive-error algs
- Good worst-case analysis
- No statistical analysis



Practical applications

- NLA, ML, statistics, data analysis, genetics, etc
- Fast JL transform
- Relative-error algs
- Numerically-stable algs
- Good statistical properties

How to "bridge the gap"?

- decouple randomization from linear algebra
- importance of statistical leverage scores!

Statistical leverage, coherence, etc.

Mahoney and Drineas (2009, PNAS); Drineas, Magdon-Ismail, Mahoney, and Woodruff (2012, ICML)

Definition: Given a "tall" n x d matrix A, i.e., with n > d, let U be *any* n x d orthogonal basis for span(A), & let the d-vector $U_{(i)}$ be the ith row of U. Then:

- the statistical leverage scores are $\lambda_i = ||U_{(i)}||_2^2$, for i $\varepsilon \{1,...,n\}$
- the coherence is $\gamma = \max_{i \in \{1,...,n\}} \lambda_i$
- the (i,j)-cross-leverage scores are $U_{(i)}^{T} U_{(j)} = \langle U_{(i)}, U_{(j)} \rangle$

Note: There are extension of this to:

- "fat" matrices A, with n, d are large and low-rank parameter k
- L1 and other p-norms



Randomized Numerical Linear Algebra

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Why Deep Learning Works

Local versus global

Local or small-scale properties (the proverbial needle in haystack):

- In machine learning: nearest neighbor models/rules
- In graph analytics: ego networks near a person in a social network
- This information is often the most reliable

Global or large-scale properties (the proverbial haystack):

- In machine learning: global latent factor models
- In graph analytics: large-scale community structure in social network

Algorithmic/statistical tools make strong local-global assumptions:

- Data are some large-scale structure with lots (enough to average over to go to some asymptotic limit) of small-scale noise
- Recursive spectral paritioning
- Typical ML objectives, e.g., MSE, bias toward large classes

Networks and networked data

Lots of "networked" data!!

- technological networks (AS, power-grid, road networks)
- biological networks (food-web, protein networks)
- social networks (collaboration networks, friendships)
- information networks (co-citation, blog cross-postings, advertiser-bidded phrase graphs ...)
- language networks (semantic networks ...)

Interaction graph model of networks:

- Nodes represent "entities"
- Edges represent "interaction" between pairs of entities



Possible ways a graph might look



Scatter plot of λ_2 (the "Fiedler value") for real networks



Conventional wisdom: down is good.

Question: does this plot really tell us much about these networks?

Communities, conductances, and NCPs

Let A be the adjacency matrix of G = (V, E). The *conductance* ϕ of a set S of nodes is

$$\phi(S) = \frac{\sum_{i \in S, j \notin S} A_{ij}}{\min\{A(S), A(\bar{S})\}}, \quad \text{where} \quad A(S) = \sum_{i \in S} \sum_{j \in V} A_{ij}$$

The Network Community Profile (NCP) of the graph is

$$\Phi(k) = \min_{S \subset V, |S|=k} \phi(S)$$

Just as conductance captures a Surface-Area-To-Volume, the NCP

- captures a size-resolved Surface-Area-To-Volume notion
- captures the idea of local size-resolved bottlenecks to diffusion

Three different types of real networks





(e) NCP: conductance value of best conductance set, as function of size

(f) CRP: ratio of internal to external conductance, as function of size









US-Senate

Information propagates local-to-global in different networks in different ways



Summary of lessons learned

Local-global properties of real data are very different

than practical/theoretical people implicitly/explicitly assume

Local graph algorithms (local spectral methods) were big winner

- For both algorithmic and statistical reasons
- Little design decisions made a big difference
 - Details of how deal with truncation and boundary conditions are not second-order issues when graphs are expander-like

Approximation algorithm usefulness uncoupled from theory

Often useful when they implicitly regularize

Some basics on kernels and SPSD matrices

- ▶ Given $\vec{x_1}, \ldots, \vec{x_n} \in \mathbb{R}^d$ and $\kappa : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, the $n \times n$ matrix with elements $A_{ij} = \kappa(\vec{x_i}, \vec{x_j})$ is the kernel matrix of κ w.r.t. $\vec{x_1}, \ldots, \vec{x_n}$.
 - Appropriate κ ensures A is SPSD
 - A_{ij} measure a (κ -defined) similarity between points *i* and *j*.
 - κ determines a *feature map* Φ_κ : ℝ^d → ℝ[∞] s.t. similarity of x_i and x_j in feature space is measure by A_{ij} = ⟨Φ_κ(x_i), Φ_κ(x_j)⟩.
- ▶ When κ is the usual Euclidean inner-product, so that $A_{ij} = \langle \vec{x}_i, \vec{x}_k \rangle$, then A is called a **Linear Kernel** matrix.

• **Gaussian RBF Kernel** matrices, defined by $A_{ij}^{\sigma} = \exp\left(\frac{-\|\vec{x}_i - \vec{x}_j\|_2^2}{\sigma^2}\right)$, correspond to the similarity measure $\kappa(\vec{x}, \vec{y}) = \exp(-\|\vec{x} - \vec{y}\|_2^2/\sigma^2)$.

- σ defines "size scale" over which points "see" each other.
- Can "sparsify" A by decreasing σ .
- Can also sparsify the matrix A by zeroing out entries.

Size-dependence of optimal neighbor width

Wang, Li, Mahoney, and Darve (2015)

EMG Physical Action Data Set

	10 normal	&	10	aggressive	physical	actions that	measure h	uman	activity.
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Class	1	2	3	4	5	6	7	8	9	
r _i ²	1e-4	3e-4	1.2e-3	2.8e-3	2.6e-2	2.7e-2	3.6e-2	4.6e-1	1.0	
d _i ²	3e-4	2.3e-3	9.9e-3	1.7e-2	1.9e-1	2.3e-1	1.4e-1	1.4	2.1	
Class	10	11	12	13	14	15	16	17	18	19
r _i ²	1.0	1.6	1.9	2.2	2.2	2.6	2.8	2.9	3.0	3.1
d _i ²	2.0	3.4	4.4	4.2	4.3	5.3	5.4	5.4	5.7	5.9

Table: Pair-wise distance (d_i) and distance to center (r_i) for each class

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We order the classes by their "size" r_i and group them as follows:
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g1 = smallest class,
g2 = union(smallest & 2nd smallest class),
..., g20 = all the data
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Use case¹: Galactic spectra from SDSS

 $x_i \in \mathbb{R}^{3841}, N \approx 500k$

photon fluxes in ≈ 10 Å wavelength bins

preprocessing corrects for redshift, gappy regions

normalized by median flux at certain wavelengths



¹Also results in neuroscience as well as genetics and mass spec imaging.

Global embedding: effect of k



Figure: Eigenvectors 3 and 4 of Lazy Markov operator, k = 2:2048

Global embedding: average spectra



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MOV optimization approach to local spectral methods

(Mahoney, Orecchia, and Vishnoi, 2009; Hansen and Mahoney, 2013; Lawlor, Budavari, Mahoney, 2015)

Suppose we have:

- 1. a seed vector $s = \chi_S$, where S is a subset of data points
- 2. a correlation parameter κ

MOV objective. The first semi-supervised eigenvector w_2 solves:

minimize
$$x^T L x$$

subject to $x^T D x = 1$
 $x^T D \mathbb{1} = 0$
 $x^T D s \ge \sqrt{\kappa}$

Similarly for w_t with addition constraints $x^T D w_j = 0, j < t$.

Theorem. Solution can be found by solving a linear equation. It is "quadratically good" (with a local version of Cheeger's Inequality).

Local embedding: scale parameter and effect of seed For an appropriate choice of c and $\gamma = \gamma(\kappa) < \lambda_2$, one can show

$$w_2 = c(L - \gamma D)^+ Ds$$

= $c(L_G - \gamma L_{k_n})^+ Ds$

(In practice, binary search to find "correct" γ .)



Figure: (left) Global embedding with seeds in black. (middle, right) Local embeddings using specified seeds.

Pictorial illustration of what can be discovered

Mahoney, Orecchia, and Vishnoi, (2009); Maji, Vishnoi, and Malik (2011); Hansen and Mahoney, (2013)



- Cannot find the tiger with global eigenvectors.
- Can find the tiger with our LocalSpectral method!



Randomized Numerical Linear Algebra

Structure in Social and Other Informatics Graphs

Why Deep Learning Works

Motivations: towards a Theory of Deep Learning

Theoretical: deeper insight into Why Deep Learning Works?

- convex versus non-convex optimization?
- explicit/implicit regularization?
- is / why is / when is deep better?
- VC theory versus Statistical Mechanics theory?

• . . .

Practical: use insights to improve engineering of DNNs?

- when is a network fully optimized?
- can we use labels and/or domain knowledge more efficiently?
- large batch versus small batch in optimization?
- designing better ensembles?

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• ...
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Motivations: towards a Theory of Deep Learning



Raises broad questions about Why Deep Learning Works

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Implicit Self-regularization in DNNs

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Set up: the Energy Landscape

Energy/Optimization function:

 $E_{DNN} = h_L(\mathbf{W}_L \times h_{L-1}(\mathbf{W}_{L-1} \times h_{L-2}(\cdots) + \mathbf{b}_{L-1}) + \mathbf{b}_L)$

Train this on labeled data $\{d_i, y_i\} \in \mathcal{D}$, using Backprop, by minimizing loss \mathcal{L} :

$$\min_{W_i, b_i} \mathcal{L}\left(\sum_i E_{DNN}(d_i) - y_i\right)$$

*E*_{DNN} is "the" *Energy Landscape*:

- The part of the optimization problem parameterized by the heretofore unknown elements of the weight matrices and bias vectors, and as defined by the data {d_i, y_i} ∈ D
- Pass the data through the Energy function E_{DNN} multiple times, as we run Backprop training
- The Energy Landscape* is *changing* at each epoch

*i.e., the optimization function that is *nominally* being optimized $\langle a \rangle = \langle a \rangle \langle a \rangle$

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Implicit Self-regularization in DNNs

Motivations: what is regularization?



Every adjustable *knob* and *switch*—and there are *many*[†]—is regularization.

[†]https://arxiv.org/pdf/1710.10686.pdf

How we will study regularization

The Energy Landscape is *determined* by layer weight matrices W_L :

$$E_{DNN} = h_L(\mathbf{W}_L \times h_{L-1}(\mathbf{W}_{L-1} \times h_{L-2}(\cdots) + \mathbf{b}_{L-1}) + \mathbf{b}_L)$$

Traditional regularization is applied to \mathbf{W}_L :

$$\min_{W_l, b_l} \mathcal{L}\left(\sum_i E_{DNN}(d_i) - y_i\right) + \alpha \sum_l \|\mathbf{W}_l\|$$

Different types of regularization, e.g., different norms $\|\cdot\|$, leave different empirical signatures on \mathbf{W}_L .

What we do:

- Turn off "all" regularization.
- Systematically turn it back on, explicitly with α or implicitly with knobs/switches.
- Study empirical properties of \mathbf{W}_L .

Lots of DNNs Analyzed

Question: What happens to the layer weight matrices W_L ?

(Don't evaluate your method on one/two/three NN, evaluate it on a dozen/hundred.)

Retrained LeNet5 on MINST using Keras.

Two other small models:

- 3-Layer MLP
- Mini AlexNet



Wide range of state-of-the-art pre-trained models:

• AlexNet, Inception, etc.

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Matrix complexity: Singular/Eigen Value Densities

$$\mathbf{W} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{T} \qquad \nu_{i} = \mathbf{\Sigma}_{ii} \qquad p_{i} = \nu_{i}^{2} / \sum_{i} \nu_{i}^{2}$$
$$\mathcal{S}(\mathbf{W}) = \frac{-1}{\log(R(\mathbf{W}))} \sum_{i} p_{i} \log p_{i} \qquad \mathcal{R}_{s}(\mathbf{W}) = \frac{\|\mathbf{W}\|_{F}^{2}}{\|\mathbf{W}\|_{2}^{2}} = \frac{\sum_{i} \nu_{i}^{2}}{\nu_{max}^{2}}$$



Figure: Histograms of the Singular Values ν_i and associated Eigenvalues $\lambda_i = \nu_i^2$.

Random Matrix Theory 103: Heavy-tailed RMT

Go beyond the (relatively easy) Gaussian Universality class:

• model strongly-correlated systems ("signal") with heavy-tailed random matrices.

	Generative Model	Finite-N	Limiting	Bulk edge	(far) Tail
	w/ elements from	Global shape	Global shape	Local stats	Local stats
	Universality class	$\rho_N(\lambda)$	$\rho(\lambda), N \to \infty$	$\lambda \approx \lambda^+$	$\lambda \approx \lambda_{max}$
Basic MP	Gaussian	MP distribution	MP	TW	No tail.
Spiked- Covariance	Gaussian, + low-rank perturbations	MP + Gaussian spikes	MP	TW	Gaussian
Heavy tail, $4 < \mu$	(Weakly) Heavy-Tailed	MP + PL tail	MP	Heavy-Tailed*	Heavy-Tailed*
Heavy tail, $2 < \mu < 4$	(Moderately) Heavy-Tailed (or "fat tailed")	$\sim \lambda^{-(a\mu+b)}$	$\sim \lambda^{-(\frac{1}{2}\mu+1)}$	No edge.	Frechet
Heavy tail, $0 < \mu < 2$	(Very) Heavy-Tailed	$\sim \lambda^{-(\frac{1}{2}\mu+1)}$	$\sim \lambda^{-(\frac{1}{2}\mu+1)}$	No edge.	Frechet

Basic MP theory, and the spiked and Heavy-Tailed extensions we use, including known, empirically-observed, and conjectured relations between them. Boxes marked "*" are best described as following "TW with large finite size corrections" that are likely Heavy-Tailed, leading to bulk edge statistics and far tail statistics that are indistinguishable. Boxes marked "*" are phenomenological fits, describing large ($2 < \mu < 4$) or small ($0 < \mu < 2$) finite-size corrections on $N \to \infty$ behavior.

Experiments: just apply this to pre-trained models

https://medium.com/@siddharthdas_32104/cnns-architectures-lenet-alexnet-vgg-googlenet-resnet-and-more-...

Year	CNN	Developed by	Place	Top-5 error rate	No. of parameters
1998	LeNet(8)	Yann LeCun et al			60 thousand
2012	AlexNet(7)	Alex Krizhevsky, Geoffrey Hinton, Ilya Sutskever	1st	15.3%	60 million
2013	ZFNet()	Matthew Zeiler and Rob Fergus	1st	14.8%	
2014	GoogLeNet(1 9)	Google	1st	6.67%	4 million
2014	VGG Net(16)	Simonyan, Zisserman	2nd	7.3%	138 million
2015	ResNet(152)	Kaiming He	1st	3.6%	



An Analysis of Deep Neural Network Models for Practical Applications, 2017.

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RMT: LeNet5 (an old/small example)



Figure: Full and zoomed-in ESD for LeNet5, Layer FC1.

Marchenko-Pastur Bulk + Spikes

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Implicit Self-regularization in DNNs

RMT: AlexNet (a typical modern DNN example)

 $\dot{0}$ $\dot{2}$ $\dot{4}$ Eigenvalues (λ) of $\mathbf{X} = \mathbf{W}_{EC1}^{T} \mathbf{W}_{EC1}$



Figure: Zoomed-in ESD for Layer FC1 and FC3 of AlexNet.

Marchenko-Pastur Bulk-decay + Heavy-tailed

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Eigenvalues (λ) of $\mathbf{X} = \mathbf{W}_{FC3}^T \mathbf{W}_{FC3}$



Figure: ESD for Layers L226 and L302 in InceptionV3, as distributed w/ pyTorch.

Marchenko-Pastur bulk decay, onset of Heavy Tails

RMT-based 5+1 Phases of Training



Figure: The 5+1 phases of learning we identified in DNN training.

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RMT-based 5+1 Phases of Training

We model "noise" and also "signal" with random matrices:

$$\mathbf{W} \simeq \mathbf{W}^{rand} + \Delta^{sig}. \tag{1}$$

	Operational Definition	Informal Description via Eqn. (1)	Edge/tail Fluctuation Comments	Illustration and Description
Random-like	ESD well-fit by MP with appropriate λ^+	\mathbf{W}^{rand} random; $\ \Delta^{sig}\ $ zero or small	$\lambda_{max} pprox \lambda^+$ is sharp, with TW statistics	Fig. 10(a)
Bleeding-out	ESD RANDOM-LIKE, excluding eigenmass just above λ^+	W has eigenmass at bulk edge as spikes "pull out"; Δ ^{sig} medium	$\begin{array}{c} BPP \text{ transition,} \\ \lambda_{max} \text{ and} \\ \lambda^+ \text{ separate} \end{array}$	Fig. 10(b)
Bulk+Spikes	$\begin{array}{l} ESD \mathrm{Random-Like} \\ plus \geq 1 spikes \\ well above \lambda^+ \end{array}$	\mathbf{W}^{rand} well-separated from low-rank Δ^{sig} ; $\ \Delta^{sig}\ $ larger	λ^+ is TW, λ_{max} is Gaussian	Fig. 10(c)
Bulk-decay	ESD less RANDOM-LIKE; Heavy-Tailed eigenmass above λ^+ ; some spikes	Complex ∆ ^{sig} with correlations that don't fully enter spike	Edge above λ^+ is not concave	Fig. 10(d)
Heavy-Tailed	ESD better-described by Heavy-Tailed RMT than Gaussian RMT	\mathbf{W}^{rand} is small; Δ^{sig} is large and strongly-correlated	No good λ^+ ; $\lambda_{max} \gg \lambda^+$	Fig. 10(e)
RANK-COLLAPSE	ESD has large-mass spike at $\lambda = 0$	W very rank-deficient; over-regularization	_	Fig. 10(f)

The 5+1 phases of learning we identified in DNN training.

Bulk+Spikes: Small Models



Smaller, older models can be described perturbatively with Gaussian RMT

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Bulk+Spikes: Small Models \sim Tikhonov regularization



Smaller, older models like LeNet5 exhibit traditional regularization

Heavy-tailed Self-regularization

W is *strongly-correlated* and highly non-random

• Can model strongly-correlated systems by heavy-tailed random matrices

Then RMT/MP ESD will also have heavy tails

Known results from RMT / polymer theory (Bouchaud, Potters, etc)



Larger, modern DNNs exhibit novel Heavy-tailed self-regularization

12 N 4 2 N

Heavy-tailed Self-regularization

Summary of what we "suspect" today

- No single scale threshold.
- No simple low rank approximation for \mathbf{W}_L .
- Contributions from correlations at all scales.
- Can not be treated perturbatively.

Larger, modern DNNs exhibit novel Heavy-tailed self-regularization

Implications: RMT and Deep Learning



How can RMT be used to understand the Energy Landscape?

Implications: Minimizing Frustration and Energy Funnels

As simple as can be?, Wolynes, 1997



Energy Landscape Theory: "random heteropolymer" versus "natural protein" folding

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Implications: Energy Landscapes of Heavy-tailed Models?



Compare with (Gaussian) Spin Glass model of Choromanska et al. 2015

Spin Glasses with Heavy Tails?

• Local minima do not concentrate near the ground state (Cizeau and Bouchaud 1993)

If Energy Landscape is more funneled, then no "problems" with local minima!

Conclusions

Practice:

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Theory:

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