Gaussian Complexity, Metric Entropy & Risk of Deep Nets

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Target of Investigation


- **Network Variation $V$**: Sums of weights of network paths.

- **Risk bound**: Least squares $\hat{f}$. Observations $Y_i = f(X_i) + \epsilon_i$ with (sub-)Gaussian error, sample size $n$.

  $$E[\|\hat{f} - f\|^2] \leq V \left( \frac{L + \log d'}{n} \right)^{1/2}$$

- **Precursor Work**: Neyshabur et al ('15), Golowich et al ('18), Barron & Klusowski ('18) with other complexity controls.

- **Gaussian process comparison inequalities**: Key to provide the risk bounds in current form.
Geometric width of sets

- **Arbitrary set of interest:** $A_n$ in $\mathbb{R}^n$. For statistical application
  
  $$A_n = \mathcal{F}_{x^n} = \{(f(x_1), f(x_2), \ldots, f(x_n)) : f \in \mathcal{F}\}$$

  restriction of a class $\mathcal{F}$ of functions to data $x_1, x_2, \ldots, x_n$.

- **Half space** in direction determined by $\xi = (\xi_1, \xi_2, \ldots, \xi_n)$ with threshold $t$
  
  $$\{a : \xi \cdot a \leq t\}$$

- **Half space supporting** $A_n$ in the direction determined by $\xi$
  uses the threshold
  
  $$t_n = t_n(\xi, A_n) = \sup_{a \in A_n} \xi \cdot a$$

- **Support function** $t_n(\xi, A_n)$ is "width" of $A_n$ in direction $\xi$.
  The least threshold such that the half space contains $A_n$. 
Probabilistic Geometry Width

- **Probabilistic width**: for random $\xi$ with distribution $\mu$.
- **Mean width**: The $\mu$ complexity of $A_n$
  \[
  C_\mu(A_n) = E_\xi \sup_{a \in A_n} \xi \cdot a
  \]
- **Cummulant generating function of the width**: 
  \[
  C_{\lambda,\mu}(A_n) = \frac{1}{\lambda} \log E[e^{\lambda \sup_{a \in A_n} \xi \cdot a}]
  \]
- **General width**: Positive increasing convex $g$ with inverse $\psi$
  \[
  C_{g,\mu}(A_n) = \psi(E[g(\sup_{a \in A_n} \xi \cdot a)])
  \]
- **For Rademacher Complexity**: $\xi_i$ indep symmetric Bernoulli
- **For Gaussian Complexity**: $\xi_i$ independent Gaussian
- **Some relationship**: Tomczak-Jaegermann ('89). There are positive constants $c$, $\overline{c}$ such that for all $A_n$
  \[
  c C_{Rad}(A_n) \leq C_{Gaussian}(A_n) \leq \overline{c} C_{Rad}(A_n) \log n
  \]
Random process perspective

- Random process: indexed by $a$ in $A_n$

$$Z_a = \xi \cdot a = \sum_{i=1}^{n} a_i \xi_i$$

- This $Z_a$ is of course a Gaussian process if $\xi$ is Gaussian

- Isometry: If $\xi$ has identity covariance then

$$E[(Z_a - Z_b)^2] = \|a - b\|^2$$

- Probabilistic width studies the maximum of the process

$$C_{\mu}(A_n) = E[\sup_{a \in A_n} Z_a]$$
More general error distributions: sub-Gaussian instead of bounded error

Stronger link to the metric entropy: via Sudakov and Dudley inequalities. The Sudakov lower bound can also be revealed via statistical risk and information theory analysis using Fano’s inequality.

Analogous contraction properties: Most important for our present purposes.
Gaussian Comparison Inequality

- Let $\tilde{Z}_a$ be Gaussian majorized by $Z_a$ in expectation
  \[ E[\tilde{Z}_a^2] \leq E[Z_a^2] \]
  
  and

  \[ E[(\tilde{Z}_a - \tilde{Z}_b)^2] \leq E[(Z_a - Z_b)^2] \]

- By Vitale (2000), equation 13, for increasing convex $g$,
  \[ E[g(\sup_{a \in A_n} \tilde{Z}_a)] \leq E[g(\sup_{a \in A_n} Z_a)] \]

- Refines Fernique (1975) which worked with
  \[ E[ \sup_{a, b \in A_n} (Z_a - Z_b)] \]

- Refines Slepian (1962) which assumed equality in $\ast$. 
- Avoids a factor of 2.
Contraction Inequality

- Let \( \phi \) be a contraction: Lipshitz 1 with \( \phi(0) = 0 \).
- Compare the processes:

\[
\tilde{Z}_a = \sum_i \xi_i \phi(a_i) \text{ and } Z_a = \sum_i \xi_i a_i
\]

- Satisfy the majorization inequalities:

\[
E \tilde{Z}_a^2 \leq EZ_a^2 \text{ and } E(\tilde{Z}_a - \tilde{Z}_b)^2 \leq E(Z_a - Z_b)^2
\]

since this becomes

\[
\sum (\phi(a_i) - \phi(b_i))^2 \leq \sum (a_i - b_i)^2
\]

- Consequent contraction of complexity: In Gaussian \( \xi \) case

\[
E[\sup_{a \in A_n} g(\sum \xi_i \phi(a_i))] \leq E[\sup_{a \in A_n} g(\sum \xi_i a_i)]
\]

This Gaussian complexity contraction is an extension (with different proof) of the Rademahaker complexity contraction obtained by Ledoux and Talagrand ('91), inequality (4.20).
For arbitrary set $A$ in $\mathbb{R}^n$ and a contraction $\phi$, let $\phi \circ A$ be
\[
\{(\phi(a_1), \phi(a_2), \ldots, \phi(a_n)) : a \in A\}
\]
and let $\text{conv}(\pm A)$ be the signed convex hull
\[
\{\sum w_j a_j : a_j \in A, \sum |w_j| = 1\}
\]
$A' = \text{conv}(\pm \phi \circ A)$ is the set of values realizable by a layer of a network for given original input values.

As in Neyshabur et al ('15) and Golowich et al ('18), which was for Rademachers, we have also for Gaussian complexity
\[
C(A') \leq 2C(A)
\]
and
\[
C_\lambda(A') \leq C_\lambda(A) + (\log 2)/\lambda
\]

What happens with multiple layers?
Set of input vectors: $A^0 = \{x_1, x_2, \ldots, x_d\}$ each in $R^n$.

Set of one layer network outputs: restricted to said inputs

$$A^1 = \text{conv}(\pm \phi \circ A^0)$$

Intermediate layers: preserving unit total weight variation

$$A^\ell = (A^{\ell-1})' = \text{conv}(\pm \phi \circ A^{\ell-1})$$

Set of $L$ layer networks outputs: restricted to said inputs

$$A^L = (((A^0)')' \ldots)'$$
- Assume each given $x_{i,j}$ has magnitude not exceeding 1
- Initial complexity of signed input set: $C(\pm A^0) \leq C_\lambda(\pm A^0)$.
- A familiar bound often attributed to Massart uses a cummulant generating function trick and replaces the supremum by a sum.
- Resulting complexity is not more than
  \[
  C_\lambda(\pm A^0) \leq n\lambda/2 + (1/\lambda) \log(2d)
  \]
- when optimized over $\lambda$ yields the complexity bound
  \[
  C(\pm A^0) \leq \sqrt{2n \log(2d)}.
  \]
Intermediate layer complexity: for $A^\ell = \text{conv}(\pm \phi \circ A^{\ell-1})$

$$C(A^\ell) \leq 2C(A^{\ell-1}) \quad \text{and} \quad C_\lambda(A^\ell) \leq C_\lambda(A^{\ell-1}) + (\log 2)/\lambda$$

Complexity for the class of L layer networks:

- Crude: $C(A^L) \leq 2^L C(A^0)$.
- Better: $C(A^L) \leq C_\lambda(A^L) \leq C_\lambda(A^0) + (L \log 2)/\lambda$
- Optimized Complexity bound

\[ C(A^L) \leq \sqrt{2n[L \log 2 + \log 2d]} \]

Follows Golowich et al, but now, thanks to Vitale’s comparison inequality it is seen to hold for Gaussian complexity and not just Rademacher.

- Corresponding risk: based on \( C(A^L)/n \) equal to

\[ \left( \frac{2L \log 2 + 2 \log 2d}{n} \right)^{1/2} \]
Deep net function $f(W, x)$, weights $W$, inputs $x$ in $[-1, 1]^d$, 

$$
\phi_{out}(\sum_{j_1} w_{j_1} \phi(\sum_{j_2} w_{j_1,j_2} \phi(\sum_{j_3} w_{j_2,j_3} \cdots \phi(\sum_{j_L} w_{j_{L-1},j_L} x_j)))),
$$

where $\phi_{out}$ is any specified Lipschitz(1) function.

Activation functions are $\pm$ positive part, rectified linear units

$\phi(z) = (z)_+$ for first half of nodes on each layer

$\phi(z) = -(z)_+$ for the second half.

Weights $w_{j_{\ell-1},j_\ell}$ may thus be arranged to be non-negative.

Computation at node $j_\ell$ on layer $\ell$.

$$
z_{j_\ell} = \phi(\sum_{j_{\ell+1}} w_{j_\ell,j_{\ell+1}} z_{j_{\ell+1}})
$$
Homogeneity property of positive part. For $w \geq 0$

$$w \phi(z) = \phi(wz).$$

Implication. May push weights to the innermost layer

$$f(W, x) = \sum_{j_1} \phi \left( \sum_{j_2} \phi \left( \sum_{j_3} \cdots \phi \left( \sum_{j_L} w_{j_1, j_2, \ldots, j_L} x_{j_L} \right) \right) \right).$$

Composite weights of paths $j_1, j_2, \ldots, j_L$

$$w_{j_1, j_2, \ldots, j_L} = w_{j_1} w_{j_1, j_2} w_{j_2, j_3} \cdots w_{j_{L-1}, j_L}.$$

Full network variation

$$V = \sum_{j_1, \ldots, j_L} w_{j_1, \ldots, j_L}.$$
Probabilistic Characterization of Deep Nets

- Path weights provide a joint probability distribution

\[ q_{j_1,j_2,\ldots,j_L} = \frac{W_{j_1,j_2,\ldots,j_L}}{V}. \]

- It has a Markov structure

\[ q_{j_1,j_2,\ldots,j_L} = q_{j_1} q_{j_2|j_1} q_{j_3|j_2} \cdots q_{j_L|j_{L-1}}. \]

- Probability characterization of deep net \( f(x, W) = V f(x, q) \)

\[ f(x, q) = \sum_{j_1} \phi(\sum_{j_2} \phi(\sum_{j_3} \cdots \phi(\sum_{j_L} q_{j_1,j_2,\ldots,j_L} x_{j_L}))). \]

- Iterated expectation representation, interspersed with nonlinearities

\[ \sum_{j_1} q_{j_1} \phi(\sum_{j_2} q_{j_2|j_1} \phi(\sum_{j_3} q_{j_3|j_2} \cdots \phi(\sum_{j_L} q_{j_L|j_{L-1}} x_{j_L}))). \]
Interpretation of Variation

Interpretations of the Variation $V$

- **Probabilistic**: The total variation of the measure $W = V q$ provided by the weight paths.

- **Calculus**: With one hidden layer, as in B.1991, $V$ extends the notion of bounded variation of a function on an interval (with respect to unit step functions) to functions in $\mathbb{R}^d$ (with respect to half spaces). Generalizes to variation of functions with respect to depth $L-1$ subnets.

- **Functional Analysis**: $V$ is the atomic norm of $f$ with respect to depth $L-1$ subnets.

- **Range**: For $x$ in $[-1, 1]^d$ the range of $f(x, W)$ is in $[-V, V]$.

- **Linear Algebra**: $V$ is the entry-sum of the product of the weight matrices $W_1 W_2 \cdots W_L$, where $(W_\ell)_{j_{\ell-1},j_{\ell}} = w_{j_{\ell-1},j_{\ell}}$. 
Approximate the weights $q$ by $\tilde{q}$ from a sparse set.

Draw sample, size $M$, independent from distrib $q_{j_1,j_2,\ldots,j_L}$.

Let $K_{j_1,j_2,\ldots,j_L}$ be the counts of $j_1,j_2,\ldots,j_L$, usually zero.

Let $K_{j_ℓ,j_ℓ+1}$ be the marginal counts.

Let $\tilde{a}$ be the Markov distribution on $(j_1,j_2,\ldots,j_L)$, consistent with the pairwise marginals $\tilde{q}_{j_ℓ,j_ℓ+1} = K_{j_ℓ,j_ℓ+1}/M$.

Marginals $\tilde{q}_{j_ℓ} = K_{j_ℓ}/M$.

Conditionals $\tilde{q}_{j_{ℓ+1}|j_ℓ} = K_{j_ℓ,j_{ℓ+1}}/K_{j_ℓ}$ (when $K_{j_ℓ} > 0$ and $0/0 = 0$ otherwise).

Size of set of indices $j_1,j_2,\ldots,j_L$

$$D = d_1 d_2 \cdots d_L = d^L$$

where $d$ is the geometric mean of $d_1,d_2,\ldots,d_L$. 
Log Cardinality of set of counts with specified sum $M$

$$\log\left(\frac{M+D-1}{M}\right) \leq M \log(2ed_1d_2 \cdots d_L/M) \leq ML \log d$$

At each layer, at most $M$ of the nodes can have positive weight, at most $M$ from first half and at most $M$ from second half. So when $d_\ell \geq 2M$ may replace $d_\ell$ with $d_\ell^{\text{new}} = \min\{d_\ell, 2M\}$ in representation of $f(\tilde{a}, x)$.

Refined Log Cardinality bound

$$(L-2)M \log(\min\{\bar{d}, 2M\}) + M \log(4e d_{in}),$$

where $\bar{d}$ is the geometric mean of $d_2, d_3, \ldots, d_{L-1}$.

The bound is independent of $d_1$. 
Accuracy of Deep Net Cover

- Use the $L_2(P)$ norm for any $P = P_X$ on $[-1, 1]^d$,

\[ \|f(\cdot, q) - f(\cdot, \tilde{q})\|^2 = \int (f(x, q) - f(x, \tilde{q}))^2 P_X(dx). \]

- For each $q$ there is a representor $\tilde{q}$ such that

\[ \|f(\cdot, q) - f(\cdot, \tilde{q})\| \leq C_v \frac{L}{M^{1/2}} \]

Also

\[ \|f(\cdot, q) - f(\cdot, \tilde{q})\| \leq 2 C^\text{red}_v \frac{L}{M^{1/2}} \]

- Variation coefficient

\[ C_v = \frac{1}{L} \sum_{\ell=0}^{L-1} \sum_{j_\ell} \left( V_{j_\ell}^{\text{out}} V_{j_\ell}^{\text{in}} / V \right)^{1/2} \leq \overline{V} / V^{1/2} \]

- $C^\text{red}_v$ is the same but with $V_{j_\ell}^{\text{in,red}}$ in place of $V_{j_\ell}^{\text{in}}$ with the largest incoming weighted sub-variation via $j_\ell^{*+1}$ removed.
Data Setting

- **Data**: \((X_i, Y_i), i = 1, 2, \ldots, n\)
- **Inputs**: explanatory variable vectors with arbitrary dependence
  \[X_i = (X_{i,1}, X_{i,2}, \ldots, X_{i,d})\]
- **Domain**: Cube \([-1, 1]^d\) in \(R^d\)
- **Random design**: independent \(X_i \sim P\)
- **Output**: response variable \(Y_i\) in \(R\)
  - Bounded or subgaussian
- **Relationship**: \(E[Y_i|X_i] = f(X_i)\) as in:
  - **Perfect observation**: \(Y_i = f(X_i)\)
  - **Noisy observation**: \(Y_i = f(X_i) + \epsilon_i\) with \(\epsilon_i\) indep
Statistical Risk

- Statistical risk $E\|\hat{f} - f\|^2 = E(\hat{f}(X) - f(X))^2$
- Expected squared generalization error on new $X \sim P$
- **Minimax optimal risk**, in the class $\mathcal{F}_v$ of functions with composite variation not more than $v$

\[
E\|\hat{f} - f\|^2 \leq \|f_M - f\|^2 + c\frac{1}{n} \log N(\mathcal{F}, \delta_M)
\]

with $\log N(\mathcal{F}, \delta)$ the metric entropy of $\mathcal{F}$ at $\delta_M = \|f_M - f\|$

- Achieves ideal approximation, complexity trade-off.
Statistical risk $E\|\hat{f} - f\|^2 = E(\hat{f}(X) - f(X))^2$

Expected squared generalization error on new $X \sim P$

Minimax optimal risk, in a class $\mathcal{F}$ of functions

$$E\|\hat{f} - f\|^2 \leq \|f_M - f\|^2 + c\frac{1}{n}\log N(\mathcal{F}, \delta_M)$$

with $\log N(\mathcal{F}, \delta)$ the metric entropy of $\mathcal{F}$ at $\delta_M = \|f_M - f\|$.

Specializing to the class $\mathcal{F}_\nu$ of functions with composite variation $V C^\text{red}_\nu$ not more than $\nu$

$$E\|\hat{f} - f\|^2 \leq \left(\frac{(L \nu)^2}{M}\right) + c \frac{LM \log d}{n}$$

With best $M$, our risk bound is

$$E\|\hat{f} - f\|^2 \leq 2\nu \left(\frac{c L^3 \log d}{n}\right)^{1/2}$$
Summary

- **Formulation of Deep Nets**: Positive part activation function provides weight homogeneity, probabilistic interpretation.

- **Average Variation $\overline{V}$ and Geometric Mean Variation $C_v$**: Extends notion to multi-layer nets and their sub-nets

- **Metric Entropy**: Simple log-cardinality bound $LM \log d$

- **Approximation**: Sample $M$ paths and set weights based on second order counts.

- **Approximation bound**: From telescoping control of accuracy of each layer. Bounds $C_v L/\sqrt{M}$ and $2C_v^{\text{red}} L/\sqrt{M}$.

- **Estimation**: Risk bound $C_v \left( \frac{L^3 \log d}{n} \right)^{1/2}$. From trade-off of approximation and complexity relative to the sample size $n$. 
The norm of $f$ with respect to a dictionary $G$

- **Minimal $\ell_1$ norm** on coefficients in approximation of $f$

  $$\|f\|_G = \lim_{\epsilon \to 0} \inf \{ \sum_j |c_j| : \| \sum_j c_j g_{aj} - f \| \leq \epsilon \}$$

- Also called the **variation of $f$ with respect to $G$** (B. 1991)

  $$\|f\|_G = V_G(f) = \inf \{ V : f/V \in \text{closure}(\text{conv}(\pm G)) \}$$

- Later also called the **atomic norm** of $f$ with respect to $G$
Summary

- **Flexible approximation models**
  - Subset selection
  - Nonlinearly parameterized bases as with neural nets
  - $\ell_1$ control on coefficients of combination

- **Accurate approximation with moderate number of terms**
  - Proof analogous to random coding

- **Information theoretic risk bounds**
  - Based on the minimum description length principle
  - Shows accurate estimation, even for very large dimension

- **Computational challenges are being addressed by**
  - Adaptive annealing
  - Nonlinear power methods