Computational Oracle Inequalities for Large Scale Model Selection Problems

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Observation:

For many prediction problems, the amount of data available is *effectively unlimited*.
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Information retrieval: Web search

$10^8$ websites.

$10^{10}$ pages.

$10^9$ queries/day.
Observation:
For many prediction problems, the amount of data available is effectively unlimited.

Natural language processing:
Spelling correction
Google Linguistics Data
Consortium $n$-gram corpus:
$10^{11}$ sentences.
Observation:
For many prediction problems, the amount of data available is effectively unlimited.

Computer vision: Captions
Facebook: $10^{11}$ photos.
Observation:

For many prediction problems, the amount of data available is *effectively unlimited*.

- Information retrieval: Web search
- Natural language processing: Spelling correction
- Computer vision: Captions
Observation:
For many prediction problems, performance is limited by computational resources, not sample size.

- Information retrieval: Web search
- Natural language processing: Spelling correction
- Computer vision: Captions
Example:

- Peter Norvig, “Internet-Scale Data Analysis”: On a spelling correction problem, trivial prediction rules, estimated with a massive dataset perform much better than complex prediction rules (which allow only a dataset of modest size).
- Given a limited computational budget, *what is the best trade-off?* That is, should we spend our computation on gathering more data, or on estimating richer prediction rules?
1. Computation is precious, not sample size
   - Model selection
   - Oracle inequalities

2. Computational oracle inequalities for nested hierarchies
   - Problem formulation
   - Algorithm
   - Oracle Inequality

3. Fast rates
   - Complexity regularization
   - Algorithms
   - Computational Oracle Inequalities

4. Removing the nesting assumption
   - Algorithm
   - Oracle Inequality

5. Summary and open problems
Prediction Problem

- i.i.d. \( Z_1, Z_2, \ldots, Z_n, Z \) from \( \mathcal{Z} \).
- Use data \( Z_1, \ldots, Z_n \) to choose \( \hat{f} \) from a class \( F \).
- Aim to ensure \( \hat{f} \) has small risk:

\[
L(f) = \mathbb{E} \ell(f, Z),
\]

where \( \ell : F \times \mathcal{Z} \) is a loss function.
Aim to ensure $\hat{f}$ has small risk: $L(f) = \mathbb{E}\ell(f, Z)$.

**Regression**

$$Z = (X, Y) \quad Y \in \mathbb{R},$$
$$\ell(f, Z) = (f(X) - Y)^2.$$

**Pattern Classification**

$$Z = (X, Y) \quad Y \in \{1, \ldots, m\},$$
$$\ell(f, Z) = 1[f(X) \neq Y].$$

**Density Estimation**

$$\ell(f, Z) = -\log f(Z).$$
Approximation-Estimation Trade-Off

- Define the *Bayes risk*, \( L^* = \inf_f L(f) \), where the infimum is over measurable \( f \).

- We can decompose the excess risk as
  \[
  L(\hat{f}) - L^* = \left( L(\hat{f}) - \inf_{f \in F} L(f) \right) + \left( \inf_{f \in F} L(f) - L^* \right).
  \]
  \[
  \text{estimation error} + \text{approximation error}
  \]

- Model selection: automatically choose \( F \) to optimize this trade-off.
Example 1: Norm of a linear predictor

Many linear classification algorithms minimize:

$$\min_{\theta \in \mathbb{R}^p} \sum_{i=1}^{n} \ell(y_i, \langle \theta, x_i \rangle) \quad \text{subject to} \quad \|\theta\|_2 \leq r.$$
Example 1: Norm of a linear predictor

- Many linear classification algorithms minimize:
  \[
  \min_{\theta \in \mathbb{R}^p} \sum_{i=1}^{n} \ell (y_i, \langle \theta, x_i \rangle) \quad \text{subject to} \quad \|\theta\|_2 \leq r.
  \]

- Statistical and computational complexities depend on the bound \( r \)
- Often select from a grid \( r_1 \leq r_2 \leq r_3 \leq \ldots \)
Example 2: Feature selection from an ordered set

- \( \theta \in \mathbb{R}^d \), select subset of \( \{1, 2, \ldots, d\} \) where \( \theta_i \neq 0 \)
Example 2: Feature selection from an ordered set

- $\theta \in \mathbb{R}^d$, select subset of \{1, 2, \ldots, d\} where $\theta_i \neq 0$

- Natural ordering amongst feature complexity in many problems
  - Natural language: Unigrams $\prec$ Bigrams $\prec \cdots \prec n$-grams
  - Function fitting: polynomial degree, Fourier basis dim, \ldots
  - Computer vision: hierarchy of wavelet filters

- Include features in order of complexity
Example 2: Feature selection from an ordered set

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- Natural ordering amongst feature complexity in many problems
  - Natural language: Unigrams $\prec$ Bigrams $\prec \cdots \prec n$-grams
  - Function fitting: polynomial degree, Fourier basis dim, \ldots
  - Computer vision: hierarchy of wavelet filters
- Include features in order of complexity
- Statistical and computational complexities depend on dimensionality
- Want the right number of features: $d_1 \leq d_2 \leq d_3 \leq \ldots$
Model selection over nested hierarchies

- Nested hierarchy of model classes, \( F_1 \subseteq F_2 \subseteq F_3 \subseteq \ldots \)
- Examples:
  - \( F_i = \{ \theta \in \mathbb{R}^d : \|\theta\| \leq r_i \}, \ r_1 \leq r_2 \leq r_3 \leq \ldots \)
  - \( F_i = \{ \theta \in \mathbb{R}^{d_i} : \|\theta\| \leq 1 \}, \ d_1 \leq d_2 \leq d_3 \leq \ldots \)
Model selection over nested hierarchies

- Nested hierarchy of model classes, $F_1 \subseteq F_2 \subseteq F_3 \subseteq \ldots$
- Data $Z_1, Z_2, \ldots, Z_n$

Want $i^*$ that optimizes estimation-approximation trade-off

$$L(\hat{f}_i) - L(f^*) = (L(\hat{f}_i) - \inf_{f \in F_i} L(f)) + (\inf_{f \in F_i} L(f) - L(f^*))$$

- Estimation error
- Approximation error
The Model Selection Problem

Given function classes $F_1, F_2, \ldots$, use the data $Z_1, \ldots, Z_n$ to choose $\hat{f} \in \bigcup_i F_i$ that gives a good trade-off between the approximation error and the estimation error.

Example: Complexity-penalized model selection.

\[
f^i_n = \arg \min_{f \in F_i} L_n(f),
\]

\[
\hat{f} = \text{minimizer of } L_n(f^i_n) + \gamma_i(n),
\]

where $\gamma_i(n)$ is a complexity penalty and $L_n$ is the empirical risk:

\[
L_n(f) = \frac{1}{n} \sum_{i=1}^n \ell(f, Z_i).
\]
Theorem

Suppose that we have risk bounds for each $F_i$: w.p. $1 - \delta$,

$$\sup_{f \in F_i} |L(f) - L_n(f)| \leq \gamma_i(n) + c \sqrt{\frac{\log 1/\delta}{n}}.$$ 

If $\hat{f}$ is chosen via complexity regularization:

$$f_n^i = \arg\min_{f \in F_i} L_n(f), \quad \hat{f} = \text{minimizer of } L_n(f_n^i) + \gamma_i(n),$$

then with probability $1 - \delta$,

$$L(\hat{f}) \leq \min_i \left( \inf_{f \in F_i} L(f) + 2\gamma_i(n) + c \sqrt{\frac{\log 1/\delta + \log K}{n}} \right).$$
A Simple Oracle Inequality

- Notice that, for each $F_i$ satisfying

$$
\sup_{f \in F_i} |L(f) - L_n(f)| \leq \gamma_i(n) + c \sqrt{\frac{\log 1/\delta}{n}},
$$

we have

$$
L(f_n^i) \leq \inf_{f \in F_i} L(f) + 2\gamma_i(n) + c \sqrt{\frac{\log 1/\delta}{n}}.
$$

- But complexity regularization gives $\hat{f}$ satisfying

$$
L(\hat{f}) \leq \min_i \left( \inf_{f \in F_i} L(f) + 2\gamma_i(n) + c \sqrt{\frac{\log 1/\delta + \log K}{n}} \right).
$$

- Thus, $\hat{f}$ gives a near-optimal trade-off between the approximation error and the (bound on) estimation error, with only a $\log K$ penalty.
Computation versus sample size

- Complexity regularization involves computation of the empirical risk minimizer for each $F_i$:

$$f^n_i = \arg \min_{f \in F_i} L_n(f), \quad \hat{f} = \text{minimizer of } L_n(f^n_i) + \gamma_i(n),$$

So computation typically grows linearly with $K$.

- The oracle inequality gives the best trade-off for a given sample size:

$$L(\hat{f}) \leq \min_i \left( \inf_{f \in F_i} L(f) + 2\gamma_i(n) + c \sqrt{\frac{\log 1/\delta + \log K}{n}} \right).$$
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5. Summary and open problems
Recall

$\gamma_i(n)$ is the complexity penalty for the class $F_i$ with sample size $n$. 
Scaling of penalties with computation

Recall

\( \gamma_i(n) \) is the complexity penalty for the class \( F_i \) with sample size \( n \).

Define

\( p_i(T) \) as the complexity penalty for the class \( F_i \) with computational budget \( T \).

\[
\text{computation } T \quad \Rightarrow \quad \text{sample size } n_i(T) \text{ for } F_i
\]

We set \( p_i(T) = \gamma_i(n_i(T)) \).
Define $p_i(T)$ as the complexity penalty for the class $F_i$ with computational budget $T$.

In more detail:
with computation $T$, we can ensure that, with high probability,

$$\sup_{f \in F_i} |L(f) - L_{n_i(T)}(f)| \leq \gamma_i(n_i(T)),$$

hence

$$L(f_{n_i(T)}^i) \leq \inf_{f \in F_i} L(f) + O(p_i(T)).$$
Scaling of penalties with computation

Define

\[ p_i(T) \text{ as the complexity penalty for the class } F_i \text{ with computational budget } T. \]

Our goal: A computational oracle inequality:
\( \hat{f} \) compares favorably with each model, estimated using the entire computational budget.

\[
L(\hat{f}) \leq \min_i \left( \inf_{f \in F_i} L(f) + O(p_i(T)) \right). \]

c.f. estimate \( f \) using the entire budget.
Define $p_i(T)$ as the complexity penalty for the class $F_i$ with computational budget $T$.

**Our goal:** A computational oracle inequality: $\hat{f}$ compares favorably with each model, estimated using the entire computational budget.

$$L(\hat{f}) \leq \min_i \left(\inf_{f \in F_i} L(f) + O\left(p_i \left(\frac{T}{\log T}\right)\right)\right).$$

c.f. estimate $f$ using almost the entire budget.
Naïve solution: grid search

- Allocate budget $T/K$ to each model.
- Use a sample of size $n_i(T/K)$ for $F_i$.
- Choose

$$f_{n_i}^i = \arg \min_{f \in F_i} L_{n_i}(f),$$

$$\hat{f} = \text{minimizer of } L_{n_i}(f_{n_i}^i) + \gamma_i(n_i).$$

- Satisfies oracle inequality

$$L(\hat{f}) \leq \min_i \left( \inf_{f \in F_i} L(f) + p_i \left( \frac{T}{K} \right) \right).$$
Model selection from nested classes

- Suppose that the models are ordered by inclusion:

\[ F_1 \subseteq F_2 \subseteq \cdots \subseteq F_K. \]

- Examples:
  - \( F_i = \{ f_\theta : \theta \in \mathbb{R}^d, \| \theta \| \leq r_i \} , r_1 \leq r_2 \leq \cdots \leq r_K. \)
  - \( F_i = \{ f_\theta : \theta \in \mathbb{R}^{d_i}, \| \theta \| \leq 1 \} , d_1 \leq d_2 \leq \cdots \leq d_K. \)

- Suppose that we have risk bounds for each \( F_i \): w.p. \( 1 - \delta \),

\[ \sup_{f \in F_i} |L(f) - L_n(f)| \leq \gamma_i(n) + c \sqrt{\frac{\log 1/\delta}{n}}. \]
Exploiting structure of nested classes

Want to exploit monotonicity of risks and penalties

Excess risk, $R_i^* = \inf_{f \in F_i} L(f) - L^*$:

Penalty, $\gamma_i(n)$:
Coarse grid sets

- Want to spend computation on only few classes.
- Use monotonicity to interpolate for the rest.
- Partition based on penalty values.

\[ \gamma_i(n) \]

\[ F_1, F_2, F_j, F_{j+1} \]

\[ (1 + \lambda)^j \]

\[ (1 + \lambda)^{j+1} \]
Coarse grids for model selection

Assume

1. Loss is bounded:
   \[ \ell(f, Z) \in [0, B]. \]

2. Computation grows at least linearly with sample size:
   \[ n_1(T) = O(T). \]

3. Penalty decreases no faster than \(1/n\):
   \[ \gamma_1(n) = \Omega \left( \frac{1}{n} \right). \]
Coarse grids for model selection

Then

- We can ignore $F_i$ with $\gamma_i(n_i(T)) > B$.
- We can cover all smaller classes with a coarse grid of size $s = O(\log(BT))$.

Definition (Coarse grid)

For $S \subseteq \mathbb{N}$, a set $\hat{S} \subseteq S$ is a coarse grid of size $s$ for $S$ if $|\hat{S}| = s$ and for each $i \in S$ there is an index $j \in \hat{S}$ such that

$$
\gamma_i \left( n_i \left( \frac{T}{s} \right) \right) \leq \gamma_j \left( n_i \left( \frac{T}{s} \right) \right) \leq 2 \gamma_i \left( n_i \left( \frac{T}{s} \right) \right).
$$
Coarse grids for model selection

Then

- We can ignore $F_i$ with $\gamma_i(n_i(T)) > B$.
- We can cover all smaller classes with a coarse grid of size $s = O(\log(BT))$.

- Include a new class only after penalty increases sufficiently.
- $s = \log \left( \frac{B}{\gamma_1(n_1(T))} \right) = O(\log BT)$ suffices.
Complexity regularization on a coarse grid

Given a coarse grid \( \hat{S} \) with cardinality \( s \):

1. Allocate budget \( T/s \) to each class in \( S \).
2. Choose

\[
    f^i = \arg \min_{f \in F_i} L_n(T/s)(f)
\]

\[
    \hat{f} = \arg \min_{f \in \{f^j : j \in \hat{S}\}} L_n(T/s)(f) + \gamma_j \left( n_j \left( \frac{T}{s} \right) \right).
\]
Complexity regularization on a coarse grid

Theorem

For a nested hierarchy satisfying the uniform convergence bounds, with high probability,

\[
L(\hat{f}) \leq \min_i \left\{ \inf_{f \in F_i} L(f) + O \left( \gamma_i \left( n_i \left( \frac{T}{s} \right) \right) \right) \right\} \\
\leq \min_i \left\{ \inf_{f \in F_i} L(f) + O \left( p_i \left( \frac{T}{\log T} \right) \right) \right\}
\]

- Computational cost of model selection scales logarithmically with \( T \).
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Fast Rates

Results so far rely on uniform convergence: bounds on

$$\sup_{f \in F_i} |L(f) - L_n(f)|.$$

Typical fluctuations are of the order

$$|L(f) - L_n(f)| = O \left( \frac{1}{\sqrt{n}} \right).$$

In some cases, these rates cannot be improved, and additive penalties that scale as

$$\sup_{f \in F_i} |L(f) - L_n(f)| = \Omega \left( \frac{1}{\sqrt{n}} \right)$$

give optimal oracle inequalities.
Fast Rates

However, in many cases, we can obtain faster rates. e.g., with high probability, for all $f \in F$,

$$L(f) - L(f^*) \leq 2 (L_n(f) - L_n(f^*)) + O \left( \frac{\log n}{n} \right),$$

where $L(f^*) = \min_{f \in F} L(f)$. In these cases, choosing

$$\hat{f} = \arg \min_{f \in F} L_n(f)$$

gives $L(f) \leq L(f^*) + O(\log n/n)$.

It turns out that we can use complexity regularization to exploit these faster rates, provided the $F_i$ are ordered by inclusion.

Theorem (B., 2008)

For $F_1 \subseteq F_2 \subseteq \cdots$ and $\gamma_1(n) \leq \gamma_2(n) \leq \cdots$, if

\[
\sup_i \sup_{f \in F_i} (L(f) - L(f_i^*)) - 2 (L_n(f) - L_n(f_i^*)) - \gamma_i(n)) \leq 0,
\]
\[
\sup_i \sup_{f \in F_i} (L_n(f) - L_n(f_i^*)) - 2 (L(f) - L(f_i^*)) - \gamma_i(n)) \leq 0,
\]

then $L(\hat{f}) \leq \inf_i (L(f_i^*) + 9\gamma_i(n))$,

where $\hat{f}$ minimizes $L_n(f_n^i) + 7\gamma_i(n)/2$ and $f_i^* = \arg \min_{f \in F_i} L(f)$.
This is *striking*:

- $L_n(f_n^i)$ fluctuates on a scale $1/\sqrt{n}$.
- But adding a tiny penalty $\gamma_i(n) = O(\log n/n)$ gives $L(\hat{f})$ within $O(\log n/n)$ of the best!

The explanation: the fluctuations for different $F_i$ are correlated, because the empirical minimizers are chosen using the *same data*.
Can we obtain computational oracle inequalities with these rates?
Computational Oracle Inequalities?

Can we obtain computational oracle inequalities with these rates?

**Previous Algorithm**

Given a coarse grid $\hat{S}$ with cardinality $s$:

1. Allocate budget $T/s$ to each class in $S$.
2. Choose

\[
\hat{f} = \arg \min_{f \in \{f^i : i \in \hat{S}\}} \left( L_{n_j(T/s)}(f) + \gamma_j \left( n_j \left( \frac{T}{s} \right) \right) \right).
\]
Given a coarse grid $\hat{S}$ with cardinality $s$:

1. Allocate budget $T/s$ to each class in $S$.
2. Choose

$$f^i = \arg \min_{f \in F_i} L_{n_i}(T/s)(f)$$

$$\hat{f} = \arg \min_{f \in \{ f_i : j \in \hat{S} \}} L_{n_j}(T/s)(f) + \gamma_j \left( n_j \left( \frac{T}{s} \right) \right).$$

**Obstacle:** The oracle inequality relies on the use of the *same data*. But to best use our computational budget, we should gather *more* data for simpler classes.
Algorithm for Fast Rates

Given a coarse grid $\hat{S}$ with cardinality $s$:

1. Allocate budget $T/s$ to each class in $S$.
2. Choose
   \[
   f^i = \arg \min_{f \in F_i} L_{n_i}(T/s^2)(f)
   \]
3. Define $\hat{f}$ as the $f^i$ with the largest index $i$ such that for all smaller $j$,
   \[
   L_{n_i}(f^i) + \gamma_i(n_i) \leq \inf_{f \in F_j} L_{n_i}(f) + \gamma_j(n_i).
   \]

The same data is used in comparing $f^i$ with functions from smaller classes.
Theorem

For a nested hierarchy exhibiting fast rates, with high probability,

\[ L(\hat{f}) \leq \min_i \left\{ \inf_{f \in F_i} L(f) + O \left( p_i \left( \frac{T}{\log^2 T} \right) \right) \right\} . \]
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Heterogeneous Models

In general, the $F_i$ can be heterogeneous, not ordered by inclusion.

- Different kernels.
- Graphs in directed graphical models.
- Subsets of features.

**Key idea:** Successively allocate computational quanta online.
Multi-Armed Bandits for Model Selection

- Want class $i$ that minimizes

$$\inf_{f \in F_i} L(f) + \gamma_i(n_i(T)).$$

- Use idea of *optimism in the face of uncertainty*: neatly trade off exploration and exploitation by choosing the class with the smallest lower bound on the criterion.
Want class $i$ that minimizes

$$\inf_{f \in F_i} L(f) + \gamma_i(n_i(T)).$$

We know it suffices to choose a class $i$ to minimize

$$L_{T_n_i}(f_{T_n_i}^i) + \gamma_i(n_i(T)).$$

Use the lower confidence bound:

$$L_n(f_n^i) - \gamma_i(n) - \sqrt{\frac{\log K}{n}} + \gamma_i(n_i(T)), \quad \text{where } n \text{ is the size of the sample that we have allocated already to class } i.$$
Multi-Armed Bandits for Model Selection

- Assume $n_i(T)$ is linear in $T$: $n_i(T) = Tn_i$.
- Algorithm picks class $i_t$ with smallest lower confidence bound.
- Allocate additional sample of size $n_{i_t}$ to class $i_t$.
- Regret analysis of upper-confidence-bound algorithm (Auer et al., 2002) extends to give oracle inequalities.
Oracle inequality under separation assumption

Define $\hat{i} = \arg\min_i \left( \inf_{f \in F_i} L(f) + \gamma_i(Tn_i) \right)$,

$$\Delta_i = \inf_{f \in F_i} L(f) + \gamma_i(Tn_i) - \left( \inf_{f \in F_i} L(f) + \gamma_i^*(Tn_i^*) \right).$$

Assume $\gamma_i(n) = \frac{c_i}{\sqrt{n}}$.

Theorem

Let $T_i(T)$ be the number of times class $i$ is queried. There are constants $C, \kappa_1, \kappa_2$ such that with probability at least $1 - \frac{\kappa_1}{TK^4}$,

$$T_i(T) \leq \frac{C}{n_i} \left( \frac{c_i + \kappa_2 \sqrt{\log T}}{\Delta_i} \right)^2.$$
Oracle inequality under separation assumption

Define $i^* = \arg\min_i \left( \inf_{f \in F_i} L(f) + \gamma_i(Tn_i) \right)$, 

$$\Delta_i = \inf_{f \in F_i} L(f) + \gamma_i(Tn_i) - \inf_{f \in F_i^*} L(f) + \gamma_i^*(Tn_i^*)$$.

- If we can incrementally update the choice $f^i_n$, then the fraction of budget that is assigned to a suboptimal class $i$ is no more than $\log T/(n_i T \Delta_i^2)$.
- This is essentially optimal (Lai and Robbins, 1985).
Oracle inequality without separation

- Assume that functions in \( \{F_i\} \) map to a vector space, and the loss \( \ell(\cdot, z) \) is convex.
- Define \( \hat{f} = \frac{1}{T} \sum_{t=1}^{T} f_t \), where algorithm produces \( f_t \in F_{i_t} \) at time \( t \).

**Theorem**

There is a constant \( \kappa \) such that with probability at least \( 1 - \frac{2\kappa}{TK^3} \)

\[
L(\hat{f}) = \inf_{i \in \{1, \ldots, K\}} \left( \inf_{f \in F_i} L(f) + \gamma_i(Tn_i) \right) + O\left( \sqrt{\frac{K \max\{\log T, \log K\}}{T}} \right).
\]

- Linear dependence on \( K \).
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Open problems

- For nested hierarchies, the analysis relied on a coarse multiplicative cover of the penalty values. If the penalties are data-dependent, when is this approach possible?
- What other structures on function classes lead to good computational oracle inequalities?
Summary

- For large-scale problems, data is cheap but computation is precious.
- Computational oracle inequalities for model selection: select a near-optimal model without wasting much computation on other models.
- A *nested* complexity hierarchy ensures cost logarithmic in computational budget.
- Faster rates are sometimes possible: More complicated complexity regularization schemes ensure cost polylogarithmic in computational budget.
- If not nested, cost of model selection is linear in size of hierarchy.