Computational Oracle Inequalities for Large Scale Model Selection Problems

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Joint work with Alekh Agarwal, John Duchi and Clément Levrard.

Large Scale Data Analysis

Observation:

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

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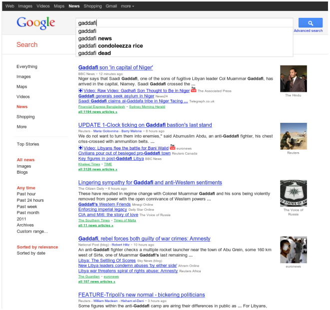
Information retrieval: Web search

10^8 websites.

10^{10} pages.

10^9 queries/day.



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Natural language processing:
Spelling correction
Google Linguistics Data Consortium n-gram corpus: 10^{11} sentences.

Large Scale Data Analysis

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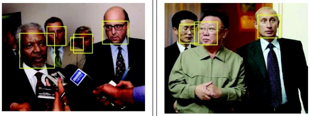
Computer vision: Captions

Facebook:

10^{11} photos.



United Nations Secretary General **Kofi Annan** stands with U.N. Security Council President and U.S. Ambassador to the U.N. **John D. Negroponte** as Annan . . .

North Korean leader **Kim Jong Il**, and Russian President **Vladimir Putin** walk after talks in Vladivostok, Friday, Aug. 23, 2002. North Korean leader Kim . . .

Large Scale Data Analysis

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

Large Scale Data Analysis

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

Large Scale Data Analysis

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?

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.

Prediction Problem: Examples

- Aim to ensure $\hat{f}$ has small *risk*: $L(f) = \mathbb{E}\ell(f, Z)$.

Regression

$$\begin{aligned} Z &= (X, Y) \qquad Y \in \mathbb{R}, \\ \ell(f, Z) &= (f(X) - Y)^2 . \end{aligned}$$

Pattern Classification

$$\begin{aligned} Z &= (X, Y) \qquad Y \in \{1, \ldots, m\}, \\ \ell(f, Z) &= 1\,[f(X) \neq Y] . \end{aligned}$$

Density Estimation

$$\ell(f, Z) = -\log f(Z).$$

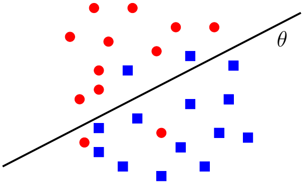
Approximation-Estimation Trade-Off

- Define the *Bayes risk*, $L^* = \inf_f L(f)$, where the infimum is over measurable f.
- We can decompose the excess risk as

$$L(\hat{f}) - L^* = \underbrace{\left(L(\hat{f}) - \inf_{f \in F} L(f) \right)}_{\text{estimation error}} + \underbrace{\left(\inf_{f \in F} L(f) - L^* \right)}_{\text{approximation error}}.$$

- Model selection: automatically choose F to optimize this trade-off.

Example 1: Norm of a linear predictor



- Many linear classification algorithms minimize:

$$\min_{\theta \in \mathbb{R}^p} \sum_{i=1}^{n} \ell\left(y_i, \langle \theta, x_i \rangle\right) \quad \text{subject to} \quad \|\theta\|_2 \leq r.$$

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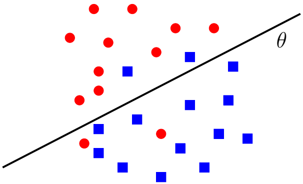

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$$\min_{\theta \in \mathbb{R}^p} \sum_{i=1}^{n} \ell\left(y_i, \langle \theta, x_i \rangle\right) \quad \text{subject to} \quad \|\theta\|_2 \leq r.$$

- 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 $\theta_i \neq 0$

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  - Natural language: Unigrams $\prec$ Bigrams $\prec \cdots \prec$ n-grams
  - Function fitting: polynomial degree, Fourier basis dim, ...
  - Computer vision: hierarchy of wavelet filters
- Include features in order of complexity

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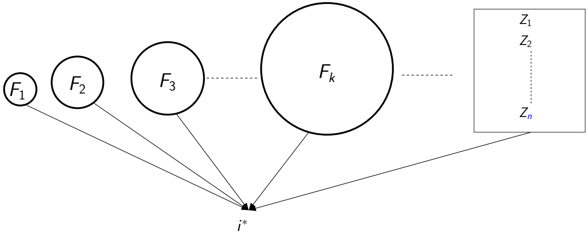
    - Function fitting: polynomial degree, Fourier basis dim, ...
    - Computer vision: hierarchy of wavelet filters
- Include features in order of complexity
- Statistical and computational complexities depend on dimensionality
- Want the right number of features: $d_1 \leq d_2 \leq d_3 \leq \ldots$

Model selection over nested hierarchies

- Nested hierarchy of model classes, $F_1 \subseteq F_2 \subseteq F_3 \subseteq \dots$
- Examples:
    - $F_i = \{\theta \in \mathbb{R}^d \ : \ \|\theta\| \le r_i\}$, $r_1 \le r_2 \le r_3 \le \dots$
    - $F_i = \{\theta \in \mathbb{R}^{d_i} \ : \ \|\theta\| \le 1\}$, $d_1 \le d_2 \le d_3 \le \dots$

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

$$L(\hat{f}_i) - L(f^*) = \underbrace{\left(L(\hat{f}_i) - \inf_{f \in F_i} L(f)\right)}_{\text{Estimation error}} + \underbrace{\left(\inf_{f \in F_i} L(f) - L(f^*)\right)}_{\text{Approximation error}}$$

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.*

$$f_n^i = \arg\min_{f \in F_i} L_n(f),$$

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

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

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

A Simple Oracle Inequality

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:

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

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:

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

  So computation typically grows *linearly with* K.

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

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

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

Scaling of penalties with computation

Recall

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

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Define

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

$$\text{computation } T \implies \text{sample size } n_i(T) \text{ for } F_i$$

We set $p_i(T) = \gamma_i(n_i(T))$.

Scaling of penalties with computation

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,

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

hence

$$L(f^i_{n_i(T)}) \leq \inf_{f \in F_i} L(f) + O(p_i(T)).$$

Scaling of penalties with computation

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.

$$L(\hat{f}) \leq \min_i \left(\underbrace{\inf_{f \in F_i} L(f) + O(p_i(T))}_{\text{c.f. estimate } f \text{ using the entire budget}} \right).$$

Scaling of penalties with computation

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.

$$L(\hat{f}) \leq \min_i \left(\underbrace{\inf_{f \in F_i} L(f) + O\left(p_i\left(\frac{T}{\log T}\right)\right)}_{\text{c.f. estimate } f \text{ using almost the entire budget}} \right).$$

Naïve solution: grid search

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

$$
\begin{aligned}
f^i_{n_i} &= \arg\min_{f \in F_i} L_{n_i}(f), \\
\hat{f} &= \text{minimizer of } L_{n_i}(f^i_{n_i}) + \gamma_i\,(n_i)\,.
\end{aligned}
$$

- 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:

$$F_1 \subseteq F_2 \subseteq \cdots \subseteq F_K.$$

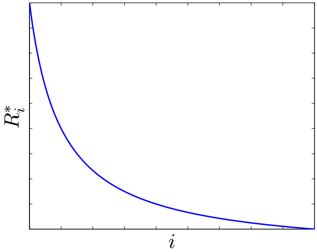
- Examples:
  - $F_i = \left\{ f_\theta : \theta \in \mathbb{R}^d, \ \|\theta\| \leq r_i \right\}, r_1 \leq r_2 \leq \cdots \leq r_K.$
  - $F_i = \left\{ f_\theta : \theta \in \mathbb{R}^{d_i}, \ \|\theta\| \leq 1 \right\}, d_1 \leq d_2 \leq \cdots \leq d_K.$
- Suppose that we have risk bounds for each F_i: w.p. $1 - \delta$,

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

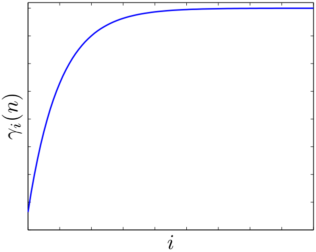
Exploiting structure of nested classes

Want to exploit monotonicity of risks and penalties

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

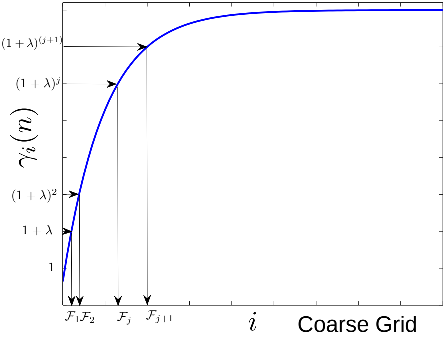


Penalty, $\gamma_i(n)$:



Coarse grid sets

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



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

$$\gamma_i\left(n_i\left(\frac{T}{s}\right)\right) \le \gamma_j\left(n_i\left(\frac{T}{s}\right)\right) \le 2\gamma_i\left(n_i\left(\frac{T}{s}\right)\right).$$

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.
- $s = \log\left(\frac{B}{\gamma_1(n_1(T))}\right) = O\left(\log BT\right)$ 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

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

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

Complexity regularization on a coarse grid

Theorem

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

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

- *Computational cost of model selection* scales logarithmically with T.

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 $f \in F$,

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

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

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

gives $L(f) \leq L(f^*) + O(\log n/n)$.
Examples: Convex losses [Lee, B., Williamson, 1998; B., Jordan, McAuliffe, 2006], classification with low noise [Mammen and Tsybakov, 2004; Tsybakov, 2004].

Oracle Inequalities with Fast Rates for Complexity Regularization

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*

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

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

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

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

Oracle Inequalities with Fast Rates for Complexity Regularization

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*.

Computational Oracle Inequalities?

Can we obtain computational oracle inequalities with these rates?

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Previous Algorithm

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

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

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

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

Computational Oracle Inequalities?

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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.

Computational Oracle Inequalities

Theorem

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

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

Heterogeneous Models

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

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

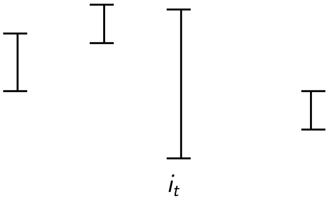
Key idea: Successively allocate computational quanta online.

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.



Multi-Armed Bandits for Model Selection

- 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

$$L_{Tn_i}(f^i_{Tn_i}) + \gamma_i(n_i(T)).$$

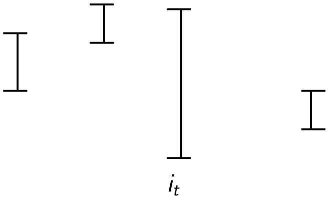
- Use the lower confidence bound:

$$L_n(f^i_n) - \gamma_i(n) - \sqrt{\frac{\log K}{n}} + \gamma_i(n_i(T)),$$

where n 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

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

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

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

Theorem

Let $T_i(T)$ be the number of times class i is queried. There are constants C, κ_1, κ_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

$$\text{Define } i^* = \arg\min_i \left(\inf_{f \in F_i} L(f) + \gamma_i(Tn_i) \right),$$
$$\Delta_i = \inf_{f \in F_i} L(f) + \gamma_i(Tn_i) - \inf_{f \in F_{i*}} L(f) + \gamma_{i^*}(Tn_{i^*}).$$

- If we can *incrementally update* the choice f_n^i, 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 κ 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.

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.