Machine Learning Theory

Lecture 11: Covering Numbers

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May 24, 2024

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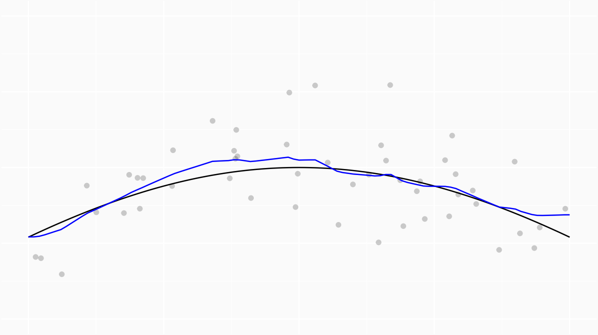
Review

Least squares with gaussian noise

We observe $Y_i = \mu(X_i) + \epsilon_i$ for $\epsilon_i \overset{iid}{\sim} N(0, \sigma^2)$.



We've focused on least squares estimators. That's the curve in your regression model that minimizes mean squared prediction error.

$$\hat{\mu} = \operatorname*{argmin}_{m \in \mathcal{M}} \frac{1}{n} \sum_{i=1}^{n} \{ Y_i - m(X_i) \}^2$$

Least squares with gaussian noise

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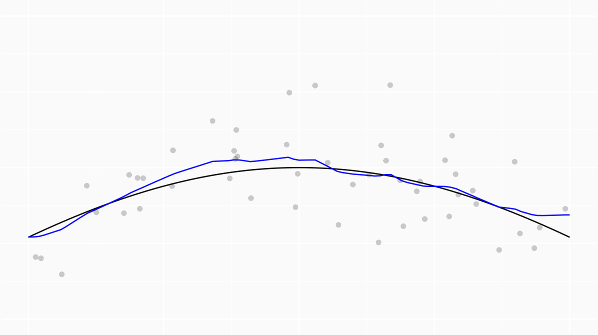

To think about how well this works, we've proven high probability bounds on the error.

$\|\hat{\mu} - \mu\| < s$ with probability $1 - \delta$ where usually $\|v\|^2 = \frac{1}{n}\sum_{i=1}^{n} v(X_i)^2$

We've mostly talked about this error's *sample two norm*.

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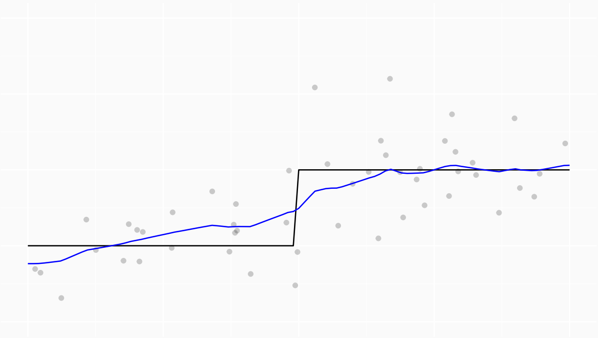
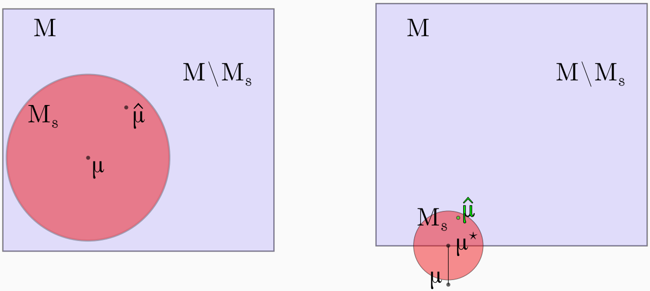


Or, more generally, on norms of the difference between our estimator and the model's best *approximation* to μ.

$\lVert \hat{\mu} - \mu^\star \rVert < s$ with probability $1 - \delta$ where $\mu^\star = \operatorname*{argmin}_{m \in \mathcal{M}} \lVert m - \mu \rVert$

What determines these bounds

It's the gaussian width of *neighborhoods* of this best approximation $\mu^\star$.



In convex models, we can work with the width of neighborhood's *boundary*.
And the bound *does not* depend on how good our approximation $\mu^\star$ is.

$$\|\hat{\mu} - \mu^\star\| < s \quad \text{w.h.p. if} \quad s^2 \geq 2\sigma c_\delta \, \mathrm{w}(\mathcal{M}_s^\circ)$$

where

$$\mathcal{M}_s^\circ = \{m \in \mathcal{M} : \|m - \mu^\star\| = s\}.$$

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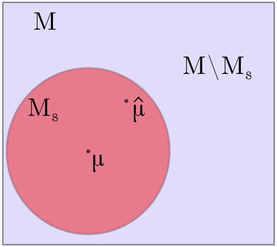
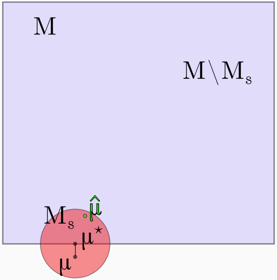




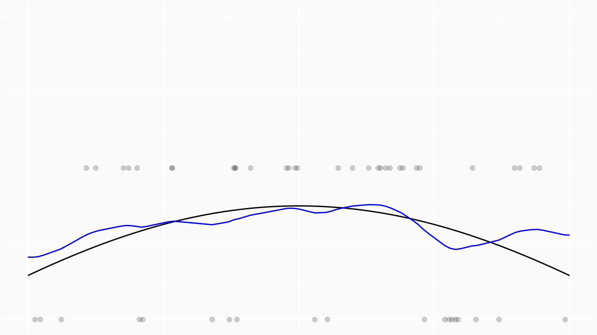
More generally, we work with the width of the neighborhood itself.
And the bound can depend on the quality of our approximation.

$$\|\hat{\mu} - \mu^\star\| < s \quad \text{w.h.p. if} \quad s^2 \geq 2\sigma c_\delta \, \mathrm{w}(\mathcal{M}_s) + 2\|\mu^\star - \mu\|$$

where

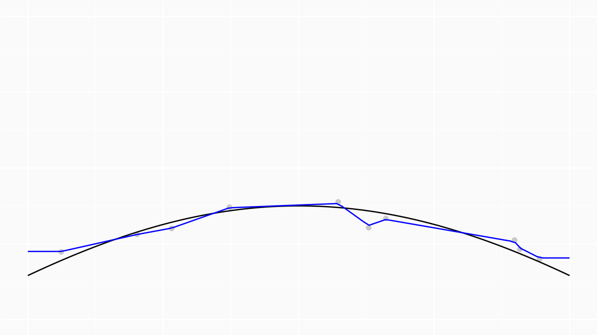
$$\mathcal{M}_s = \{m \in \mathcal{M} : \|m - \mu^\star\| \leq s\}.$$

These bounds more or less work with non-gaussian noise, too.
For example, bounded noise like what we get in *probabilistic classification*



Generalization–Population Squared Error

Same deal when we're interested in the population two-norm of our error.
Sampling from our population acts like subgaussian noise.



To use this, we need to bound gaussian width

We've done this in a few models using specialized techniques.

1. Finite models using the Union Bound and the Gaussian Tail Bound.
$$s^2 \geq cs\sqrt{\log(K)/n} \quad \text{for} \quad s \geq c\sqrt{\log(K)/n}$$
2. Finite-dimensional models using Projection and the Cauchy-Schwarz Inequality.
$$s^2 \geq s\sqrt{K/n} \quad \text{for} \quad s \geq \sqrt{K/n}$$
3. Sobolev models using Fourier Analysis and the Cauchy-Schwarz Inequality.
$$s^2 \geq cs^{1-d/2p}/\sqrt{n} \quad \text{for} \quad s \geq c'n^{-1/(2+d/p)}$$

There are two essential ideas here.

1. Approximating many curves by combinations of a few.
2. Counting.

This week, we'll talk about a completely general technique for bounding width.
We'll use the same two ideas, but our approximations will be subtler.

Finite Approximations and Gaussian Width

Finite Models

- In finite models, bounding width is easy.
- It's the maximum of gaussians with standard deviation $\le s/\sqrt{n}$.

$$
\begin{aligned}
\mathrm{E}\langle g, m-\mu^\star\rangle^2 &= \mathrm{E}\left(\frac{1}{n}\sum_{i=1}^n g_i\{m(X_i)-\mu^\star(X_i)\}\right)^2 \\
&= \frac{1}{n^2}\sum_{i=1}^n \mathrm{E}\, g_i^2\{m(X_i)-\mu^\star(X_i)\}^2 = \frac{\|m-\mu^\star\|^2}{n}.
\end{aligned}
$$

Q: What happened to the cross terms in the square?

- We can bound this via union bound. It's down to counting the curves in the model.

$$\mathrm{w}(\mathcal{M}_s) \le cs\sqrt{\frac{\log(K)}{n}} \quad \text{if } \mathcal{M} \text{ contains } K \text{ curves } v_1 \ldots v_K\text{, all with} \quad \|v-\mu^\star\|_{L_2(\mathrm{P_n})} \le s.$$

- We may be overcounting. This bounds the max of K totally different gaussians.
- That's kind of the worst case, so if there's correlation we're overcounting.
- And our gaussians are as correlated as the curves in our neighborhood.

$$\mathrm{E}\langle g, v_k\rangle\langle g, v_{k'}\rangle = n^{-2}\,\mathrm{E}\, v_k^T g g^T v_{k'} = n^{-2}\ v_k^T \underbrace{(\mathrm{E}\, gg^T)}_{I} v_{k'} = n^{-1}\ \langle v_k, v_{k'}\rangle.$$

- This definitely won't work for models with infinitely many curves.
- How do we take advantage of this correlation to tackle infinite models?

$$\mathrm{w}(\mathcal{M}_s) = \mathrm{E} \max_{v \in \mathcal{M}_s} \langle g, v \rangle \quad \text{for} \quad g \sim N(0, I_{n \times n}).$$

The difference between many of these gaussians $\langle g, v \rangle$ will be small.

- So small, sometimes, that we don't need to 'pay probability' to bound them all using the union bound. They needn't contribute to K.
- We can just use the Cauchy-Schwarz inequality to bound differences.

$$|\langle g, u \rangle - \langle g, v \rangle| = |\langle g, u - v \rangle| \leq \|g\| \|u - v\| \approx \|u - v\|.$$

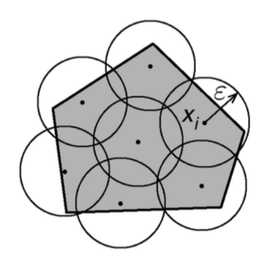
If the curves u and v are *close enough*, by bounding $\langle g, u \rangle$, we bound $\langle g, v \rangle$ *for free*.

- This means we can take K above to be smaller than the total number of curves.
- It's enough that some set $u_1 \ldots u_K$ gets close enough to all curves $v \in \mathcal{M}$.

This means we have to talk about how many *meaningfully different* curves we have.

ϵ-covers

We call a set $\mathcal{M}^\epsilon$ an ϵ-**cover** for the set $\mathcal{M}$ if every curve in the set $\mathcal{M}$ is within a distance ϵ of some curve in $\mathcal{M}^\epsilon$.



If we have an ϵ-cover $\mathcal{M}_s^\epsilon$ of size K_ϵ for $\mathcal{M}_s$, then we've got a bound on our width.

$$\begin{aligned}
\mathrm{w}(\mathcal{M}_s) &= \mathrm{E}\left[\max_{v \in \mathcal{M}_s} \langle g,\ v\rangle\right] \\
&= \mathrm{E}\left[\max_{v \in \mathcal{M}_s} \min_{u \in \mathcal{M}_s^\epsilon} \langle g,\ v-u\rangle + \langle g,\ u\rangle\right] \\
&\lesssim \underbrace{\max_{v \in \mathcal{M}_s} \min_{u \in \mathcal{M}_s^\epsilon} \|v-u\|}_{\epsilon} + \underbrace{\max_{u \in \mathcal{M}_s^\epsilon} \|u\|}_{s} \sqrt{\frac{\log(K_\epsilon)}{n}}.
\end{aligned}$$

And this works for infinite models just as well as it does for finite ones.
We can think of K_ϵ as the size of the neighborhood $\mathcal{M}_s$ at resolution ϵ.

Let’s Stop and Think

Q: Does the ϵ-cover $\mathcal{M}_s^\epsilon$ have to be a subset of $\mathcal{M}_s$ for this?

$$
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\end{aligned}
$$

Consequences

Suppose our log covering number grows like $1/\epsilon$.

$$\log(K_\epsilon) \leq \epsilon^{-1}$$

We know that $\hat{\mu}$ is in a neighborhood of $\mu^\star$ of radius s satisfying

$$s^2 \geq 2c_\delta \sigma\, \mathrm{w}(\mathcal{M}_s) \quad \text{for} \quad \mathrm{w}(\mathcal{M}_s) \leq c\epsilon + s\sqrt{\log(K_\epsilon)/n} \approx \epsilon + sn^{-1/2}\epsilon^{-1/2}$$

This width bound holds for all $\epsilon > 0$, so we can choose ϵ to minimize it.

$$0 = \frac{d}{d\epsilon}\left(\epsilon + sn^{-1/2}\epsilon^{-1/2}\right) = 1 - sn^{-1/2}\epsilon^{-3/2}/2 \quad \text{for} \quad \epsilon = \left(\frac{s}{2\sqrt{n}}\right)^{2/3} \approx s^{2/3}n^{-1/3}$$

And this tells us we're in a neighborhood of radius s like this.

$$s^2 \geq \underbrace{c\sigma s^{2/3}n^{-1/3}}_{\geq c\sigma\, \mathrm{w}(\mathcal{M}_s^\circ)} \quad \text{for} \quad s^{4/3} \geq \sigma n^{-1/3} \quad \text{i.e.} \quad s \geq \sigma^{3/4}n^{-1/4}.$$

Dissatisfying Results

- We'll show, momentarily, that $\log(K_\epsilon) \approx 1/\epsilon$ for the Lipschitz model.

$$\mathrm{w}(\mathcal{M}_s) \lesssim \epsilon + s\sqrt{\frac{\log(K_\epsilon)}{n}} \approx \epsilon + \frac{s}{\sqrt{\epsilon n}} \approx s^{2/3}n^{-1/3} \quad \text{at optimal} \quad \epsilon \approx s^{2/3}n^{-1/3}.$$

- That gives us a $n^{-1/4}$ rate.

$$s^2 \geq \mathrm{w}(\mathcal{M}_s) \quad \text{if} \quad s^2 \gtrsim s^{2/3}n^{-1/3} \quad \text{i.e. if} \quad s \approx n^{-1/4}.$$

- But we know it converges at a faster rate.
- The Lipschitz model is contained in the Sobolev model of order 1.
- And we proved the rate of convergence $s \approx n^{-1/3}$ for that using Fourier series.

Has the covering idea failed us?

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Has the covering idea failed us?

No. We just have to make better use of it. We'll do that next class.
When we do that, we'll see a rough connection to Fourier series.

Refined Bounds in terms of ϵ-nets

By working with ϵ-nets at different resolutions, we can prove a refined upper bound.

$$\mathrm{w}(\mathcal{M}_s^\circ) \lesssim \frac{1}{\sqrt{n}} \int_0^\infty \sqrt{\log(K_\epsilon)} d\epsilon \quad \text{where } K_\epsilon \text{ is the size of the smallest } \epsilon\text{-net for } \mathcal{M}_s^\circ.$$

This multi-resolution argument is called *chaining*.
The bound, *Dudley's Integral Bound*.

The Lipschitz Regression Case

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The Lipschitz Regression Case

$\log(K_\epsilon) = 0$ for $\epsilon > s$. Why? And $\log(K_\epsilon) \lesssim \epsilon^{-1}$ generally.

$$\mathrm{w}(\mathcal{M}_s^\circ) \leq \frac{1}{\sqrt{n}} \int_0^s \epsilon^{-1/2} d\epsilon = n^{-1/2} \epsilon^{1/2}/2 \mid_0^s = n^{-1/2} s^{-1/2}/2.$$

and consequently

$$s^2 \geq \mathrm{w}(\mathcal{M}_s^\circ) \quad \text{if} \quad s^{3/2} = n^{-1/2}/2 \quad \text{i.e.} \quad s \propto n^{-1/3}$$

This approach to bounding gaussian width is almost optimal.

There's also a *lower bound*, *Sudakov's Minoration Inequality*, in terms of the size K_ϵ.

$$\mathrm{w}(\mathcal{M}_s^\circ) \gtrsim \frac{1}{\sqrt{n}} \max_{\epsilon > 0} \epsilon \sqrt{\log(K_\epsilon)}.$$

These bounds are close: the upper bound is no more than $\log(n)$ times the lower.

Summary

The accuracy of our estimator is determined by the rate at which the gaussian width of our model's neighborhood boundary grows.

$$\|\hat{\mu} - \mu^\star\| < s \quad \text{with high probability} \quad \text{if} \quad s^2 \gtrsim \sigma \, \mathrm{w}(\mathcal{M}_s^\circ).$$

That gaussian width is a measure of the boundary's size at multiple resolutions.

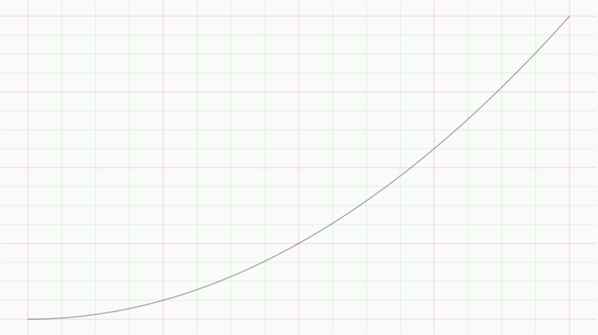
$$\frac{1}{\sqrt{n}} \max_{\epsilon > 0} \epsilon \sqrt{\log(K_\epsilon)} \underset{\lesssim}{\approx} \mathrm{w}(\mathcal{M}_s^\circ) \underset{\lesssim}{\approx} \frac{1}{\sqrt{n}} \int_0^\infty \sqrt{\log(K_\epsilon)} d\epsilon.$$

Finite Approximations and Gaussian Width

Bounding Our Covering Number in the Lipschitz Model

- Think of an ϵ-cover of $\mathcal{U}$ as the set of ϵ-approximations $\pi(u)$ for each u in $\mathcal{U}$.
- Often we base these approximations on a grid. Let's do the $1-$ Lipschitz case.

$$\mathcal{U} = \{u : |u(x') - u(x)| \leq |x' - x|,\ |u(x)| \leq 1\}.$$



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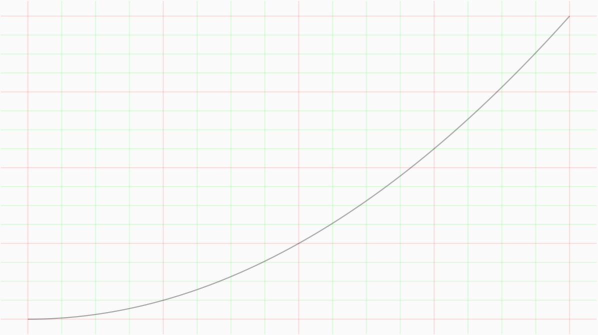

1. Draw an ϵ-spaced grid.
2. At each x-coordinate on the grid, snap to the closest grid point.
3. Because our function is 1-Lipschitz, it can't jump by more than ϵ between points.

How many of these are there? Consider $\epsilon = 1/M$ for an integer M.

$$\text{(starting points)} \cdot \text{(options per step)}^{\text{steps}} = 1/\epsilon \cdot 2^{1/\epsilon}.$$

Credit

Some things borrowed from Vershynin's *High Dimensional Probability*.

- The presentation of the refined bounds
- The ϵ-net picture.

Its chapters 7-8 are a good, although relatively sophisticated, reference for this stuff.