

Machine Learning Theory

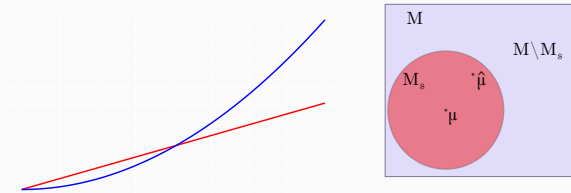
Least Squares with Sampling, Misspecification, and Non-Gaussian Noise

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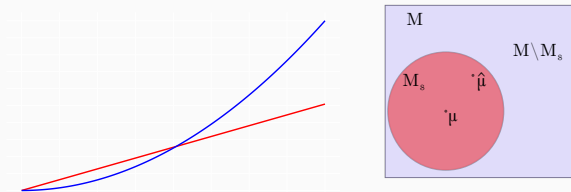
Where We Left Off



What do we know about the error of this least squares estimator $\hat{\mu}$?

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

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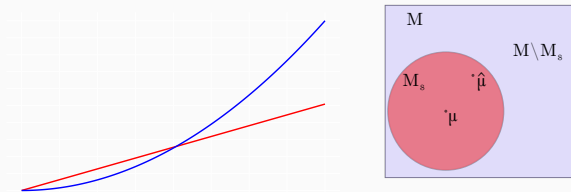
Here's what we proved in lecture.

$$\|\hat{\mu} - \mu^*\|_{L_2(P_n)} < s \quad \text{w.p. } 1 - \delta \quad \text{for} \quad \frac{s^2}{2\sigma} \geq \mathbf{w}(\mathcal{M}_s^\circ) + s \sqrt{\frac{2\Sigma_n}{\delta n}}$$

where $\mathbf{w}(\mathcal{V}) = \mathbb{E} \max_{v \in \mathcal{V}} \langle g, v \rangle_{L_2(P_n)}$ and $\Sigma_n = \sigma^2 \{1 + 2 \log(2n)\}$ for $g_i \stackrel{iid}{\sim} N(0, 1)$

if $Y_i = \mu(X_i) + \varepsilon_i$ for $\varepsilon_i \stackrel{iid}{\sim} N(0, \sigma^2)$ for $\mu \in \mathcal{M}$

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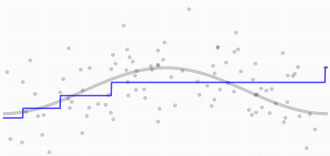
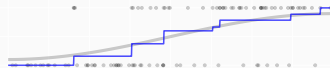
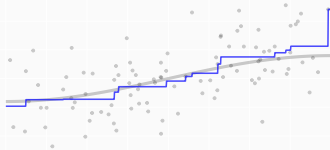
Here's a simplified version of you're proving for homework.

$$\|\hat{\mu} - \mu^*\|_{L_2(P_n)} < s + 2\sqrt{\frac{2\Sigma_n}{\delta n}} \quad \text{w.p. } 1 - \delta \quad \text{for } \frac{s^2}{2\sigma} \geq \mathbf{w}(\mathcal{M}_s)$$

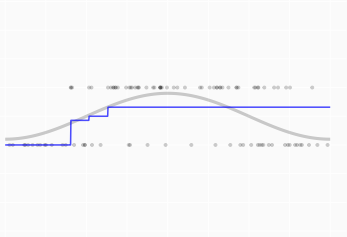
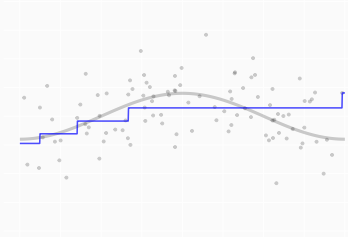
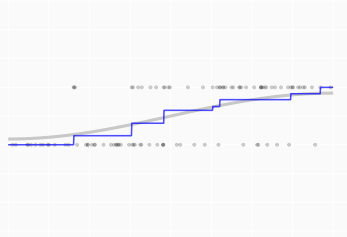
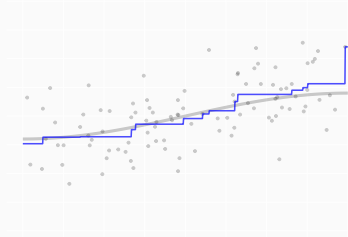
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When Does This Bound Apply?

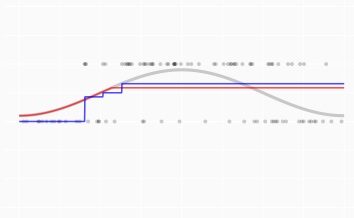
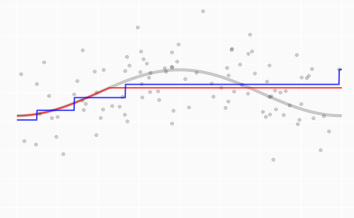
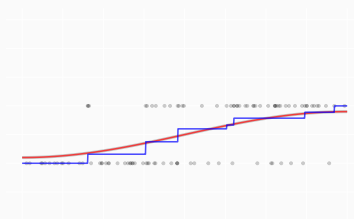
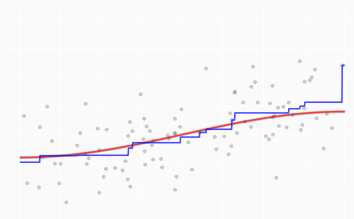


When Does This Bound Apply?

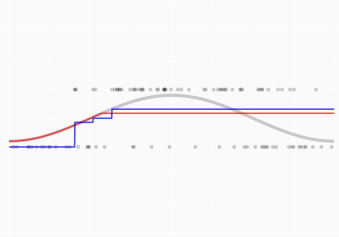
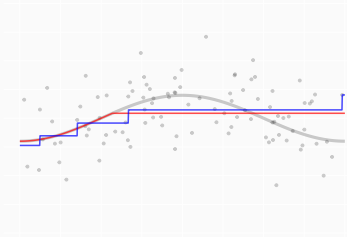
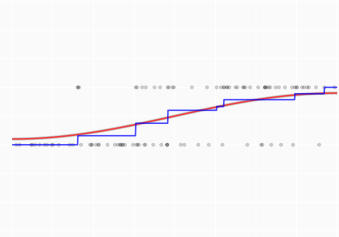
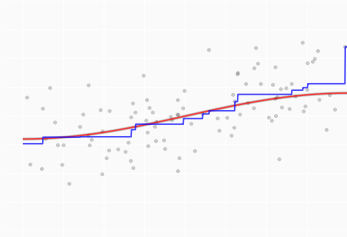


- The second column is out. We've assumed correct specification.
- The second row is out. We've assumed normality.

Today, We Fix That



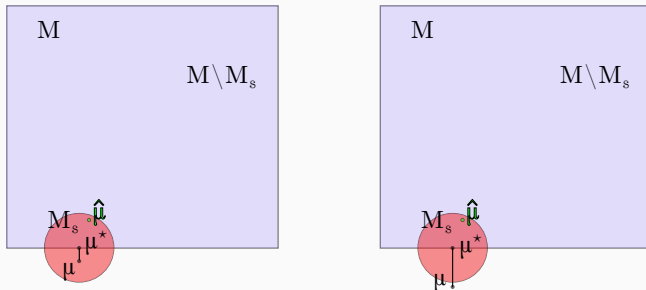
Today, We Fix That



- With misspecification, we estimate the model's **best approximation** to μ .
- Non-normality doesn't really matter much. We'll look at how it affects our bound.

Misspecification

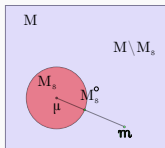
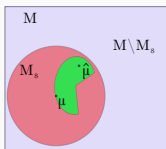
What happens when μ isn't in the model?



- Our error in estimating μ is bounded by a sum of two terms.
 - The critical radius s , i.e., the one satisfying $s^2/2\sigma \geq w(\mathcal{M}_s^\circ) + s\sqrt{\frac{2\Sigma n}{\delta n}}$.
 - The distance from μ to its best approximation in the model. Or really 3 times that.

We showed this in the model selection lab using the Cauchy-Schwarz inequality.

- In convex models, we can say more.
Our error in estimating μ^* does not depend on its distance to μ .



$\hat{\mu}$ minimizes $\ell(m) = \frac{1}{n} \sum_{i=1}^n \{Y_i - \mu(X_i)\}^2$ squared error loss
among curves m in a convex set \mathcal{M} .

- If μ is in the model, that tells us it's **one of the curves** with loss as small as μ 's.

i.e. $m = \hat{\mu}$ satisfies $\ell(m) \leq \ell(\mu)$ if $\mu \in \mathcal{M}$.

- To prove $\hat{\mu}$ is in the neighborhood \mathcal{M}_s , we show that ...

- ...none of **these curves** is in **the neighborhood's complement** $M \setminus \mathcal{M}_s$.

$\hat{\mu} \in \mathcal{M}_s$ if $\ell(m) > \ell(\mu)$ for all $m \in \mathcal{M} \setminus \mathcal{M}_s$.

- i.e. we show the *loss difference* is strictly positive for curves in **the complement**.

- That's true if it's positive for curves on **the neighborhood's boundary** \mathcal{M}_s° .

$\ell(m) - \ell(\mu) > 0$ for all $m \in \mathcal{M} \setminus \mathcal{M}_s$ if $\ell(m) > \ell(\mu)$ for all $m \in \mathcal{M}_s^\circ$.

- And that boils down to the neighborhood's *squared radius* exceeding ...

- ...twice its boundary's *maximal inner product* with noise $\varepsilon = Y - m$.

$$\ell(m) - \ell(\mu) = s^2 - \langle Y - \mu, m - \mu \rangle \geq s^2 - 2 \max_{m \in \mathcal{M}_s^\circ} \langle Y - \mu, m - \mu \rangle \quad \text{for all } m \in \mathcal{M}_s^\circ$$

- Then we do a little probability and get our error bound.

The Argument with no if

For any $\mu^* \in \mathcal{M}$, we can expand our mean squared error difference as before.

$$\ell(m) - \ell(\mu^*) = \|m - \mu^*\|_{L_2(\mathbf{P}_n)}^2 - \frac{2}{n} \sum_{i=1}^n \varepsilon_i^* \{m(X_i) - \mu^*(X_i)\} \quad \text{for } \varepsilon_i^* = Y_i - \mu^*(X_i).$$

But our new ‘noise’ ε_i^* doesn’t have mean zero. It’s our old noise ε_i , minus something.

$$\varepsilon_i^* = \underbrace{\{Y_i - \mu(X_i)\}}_{\varepsilon_i} - \underbrace{\{\mu^*(X_i) - \mu(X_i)\}}_{\text{something}}.$$

So we can think of our mean squared error difference as having three terms:

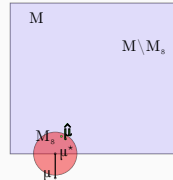
$$\begin{aligned} \ell(m) - \ell(\mu^*) &= \|m - \mu^*\|_{L_2(\mathbf{P}_n)}^2 && \text{squared distance, like before;} \\ &- \frac{2}{n} \sum_{i=1}^n \varepsilon_i \{m(X_i) - \mu^*(X_i)\} && \text{a mean zero term, like before;} \\ &+ \frac{2}{n} \sum_{i=1}^n \{\mu^*(X_i) - \mu(X_i)\} \{m(X_i) - \mu^*(X_i)\} && \text{and something else.} \end{aligned}$$

We can use our argument, ignoring the new term, if that term is always *non-negative*.

Why?

Why.

$$\begin{aligned}\ell(m) - \ell(\mu^*) &= \|m - \mu^*\|_{L_2(P_n)}^2 \\ &\quad - \frac{2}{n} \sum_{i=1}^n \varepsilon_i \{m(X_i) - \mu^*(X_i)\} \\ &\quad + \frac{2}{n} \sum_{i=1}^n \{\mu^*(X_i) - \mu(X_i)\} \{m(X_i) - \mu^*(X_i)\}\end{aligned}$$



We want to show that if distance from m to μ^* is big enough, it wins.

- In particular, it wins in the sense that the loss difference $\ell(m) - \ell(\mu^*)$ is positive.
- That implies distance from $\hat{\mu}$ to μ^* is smaller, as distance doesn't win in that case.

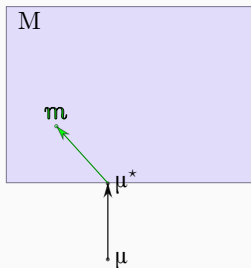
If this new term is non-negative, it helps distance win.

- If the loss difference is positive when we ignore a non-negative term ...
- ...then it's still positive when we don't.

$$\begin{aligned}\ell(m) - \ell(\mu^*) > 0 \quad \text{if} \quad & \|m - \mu^*\|_{L_2(P_n)}^2 - \frac{2}{n} \sum_{i=1}^n \varepsilon_i \{m(X_i) - \mu^*(X_i)\} > 0 \quad \text{what we're used to} \\ \text{and} \quad & \frac{2}{n} \sum_{i=1}^n \{\mu^*(X_i) - \mu(X_i)\} \{m(X_i) - \mu^*(X_i)\} \geq 0 \quad \text{new term}\end{aligned}$$

This only works if the new term is non-negative. Can we choose $\mu^* \in \mathcal{M}$ so it is?

We can



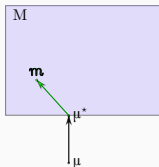
The new term is always non-negative when we compare to the *best approximation* to μ in the model,

$$\mu^* = \operatorname{argmin}_{m \in \mathcal{M}} \|m - \mu\|_{L_2(\mathcal{P}_n)}^2 \quad \text{satisfies} \quad \frac{2}{n} \sum_{i=1}^n \{\mu^*(X_i) - \mu(X_i)\} \{m(X_i) - \mu^*(X_i)\}$$

or in vector notation $\frac{2}{n} \langle \mu^* - \mu, m - \mu^* \rangle_2 \geq 0 \quad \text{for all } m \in \mathcal{M}.$

It's proportional to the dot product between two vectors: $\mu \rightarrow \mu^*$ and $\mu^* \rightarrow m$.

- When the model \mathcal{M} is convex, these vectors are always in the same direction.
- They both point 'in' to the model. That means the dot product is non-negative.



Claim. For any convex set \mathcal{M} in an inner product space,¹

$$\mu^* = \operatorname{argmin}_{m \in \mathcal{M}} \|m - \mu\| \quad \text{satisfies}$$

$$\langle \mu^* - \mu, m - \mu^* \rangle \geq 0 \quad \text{for all } m \in \mathcal{M}.$$

Proof. Let $m_\lambda = \lambda(m - \mu^*) + \mu^*$.

$$\begin{aligned} \|m_\lambda - \mu\|^2 &= \langle \lambda(m - \mu^*) + (\mu^* - \mu), \lambda(m - \mu^*) + (\mu^* - \mu) \rangle \\ &= \lambda^2 \|m - \mu^*\|^2 + \|\mu^* - \mu\|^2 + 2\lambda \langle m - \mu^*, \mu^* - \mu \rangle. \end{aligned}$$

Because $m_\lambda \in \mathcal{M}$, it follows that this is at least as large as $\|\mu - \mu^*\|^2$, so

$$0 \leq \lambda^2 \|m - \mu^*\|^2 + 2\lambda \langle m - \mu^*, \mu^* - \mu \rangle$$

and therefore, dividing by $\lambda > 0$, that

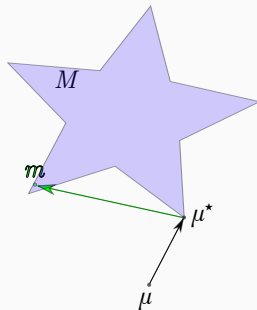
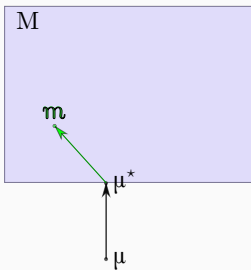
$$0 \leq \lambda \|m - \mu^*\|^2 + 2 \langle m - \mu^*, \mu^* - \mu \rangle.$$

Because this holds for arbitrarily small $\lambda > 0$, it must also hold for $\lambda = 0$.

¹An inner product space is a vector space with a norm $\|u\| = \sqrt{\langle u, u \rangle}$ induced by an inner product $\langle u, v \rangle$.

That's not true for other choices

When $\mu^* \in \mathcal{M}$ isn't the closest point to μ ,
these vectors can point in opposite directions.
That is, this dot product can be negative for some $m \in \mathcal{M}$.

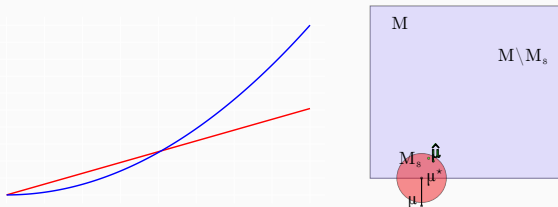


The same thing can happen *for the closest point* in a non-convex model.

Summary

When we use a convex model, the least squares estimator $\hat{\mu}$ converges to the model's closest point to μ . This generalizes our result without misspecification.

- If μ is in the model, that closest point is μ .
- Otherwise, it's something else.



We can bound our estimator's distance to that closest point μ^* just like we've been bounding distance to μ when we assumed it was in the model.

$$\|\hat{\mu} - \mu^*\|_{L_2(P_n)} < s + 2\sqrt{\frac{2\Sigma_n}{\delta n}} \text{ w.p. } 1 - \delta \text{ if } s^2/2\sigma \geq w(\mathcal{M}_s)$$

for $\mathcal{M}_s = \{m \in \mathcal{M} : \|m - \mu^*\|_{L_2(P_n)} \leq s\}$ and $\Sigma_n = \sigma\{1 + 2\log(2n)\}$

if $Y_i = \mu(X_i) + \varepsilon_i$ for $\varepsilon_i \stackrel{iid}{\sim} N(0, \sigma^2)$ for some function μ .

Misspecification

Examples

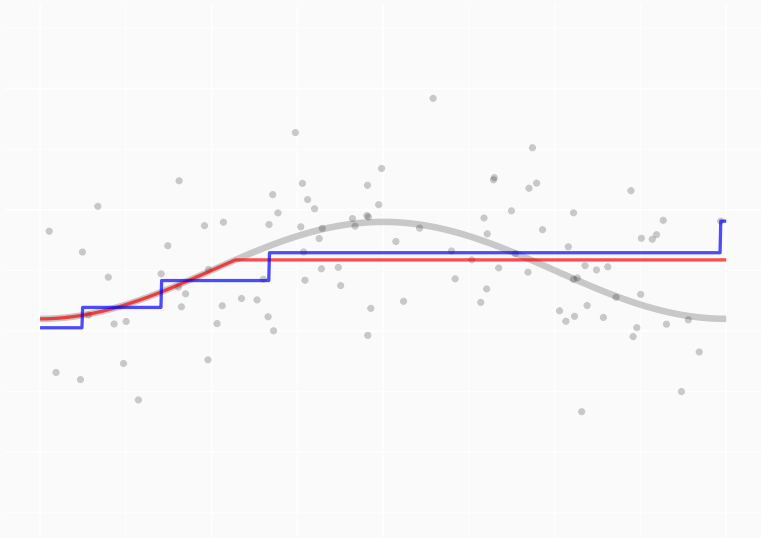


Figure 1: Increasing Curves ($n = 100$.)

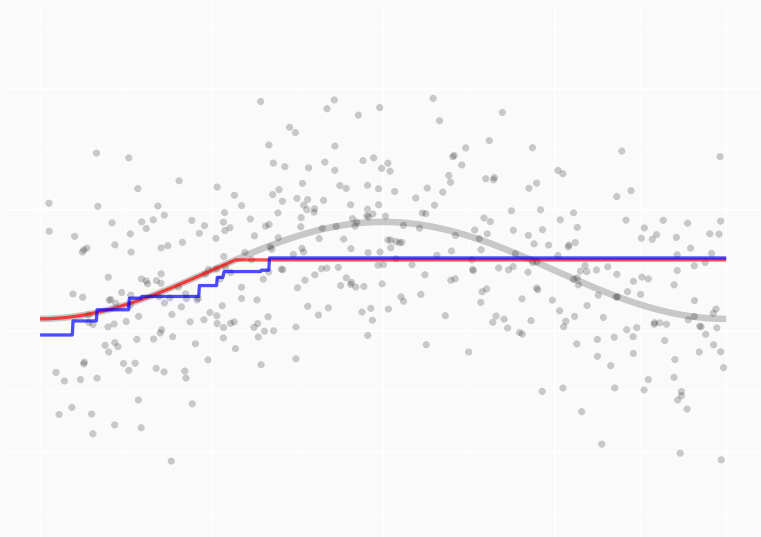


Figure 2: Increasing Curves ($n = 400$.)

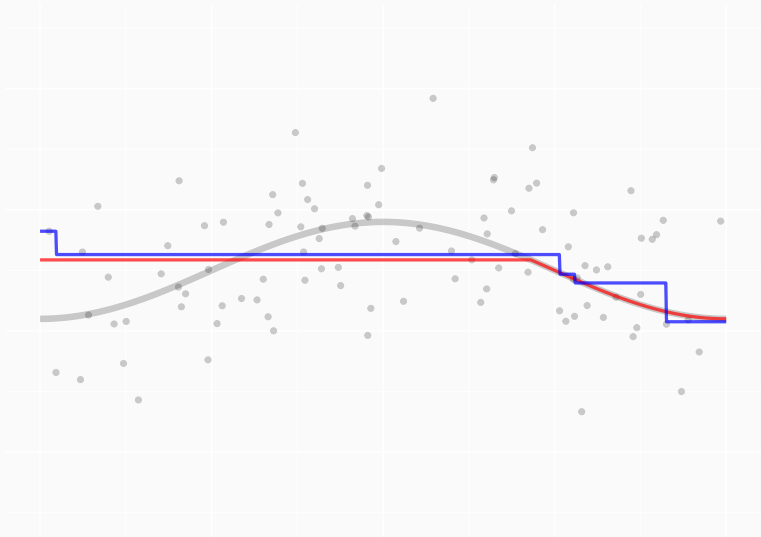


Figure 3: Decreasing Curves ($n = 100$.)

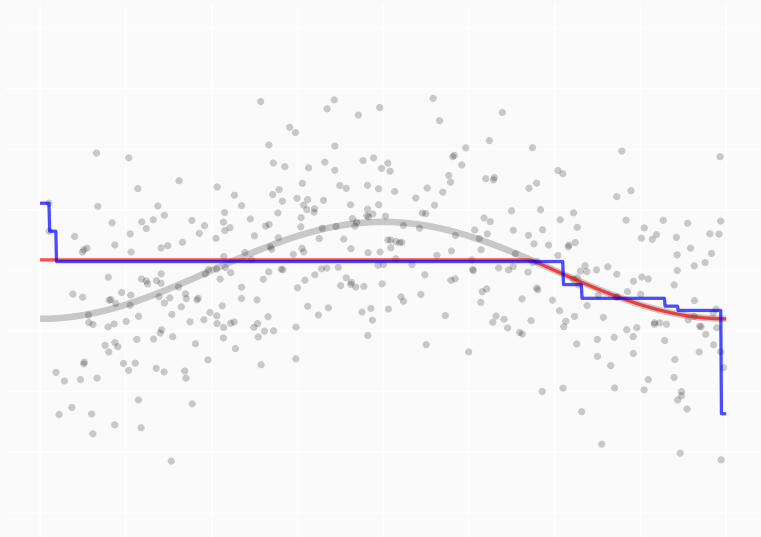


Figure 4: Decreasing Curves ($n = 400$.)

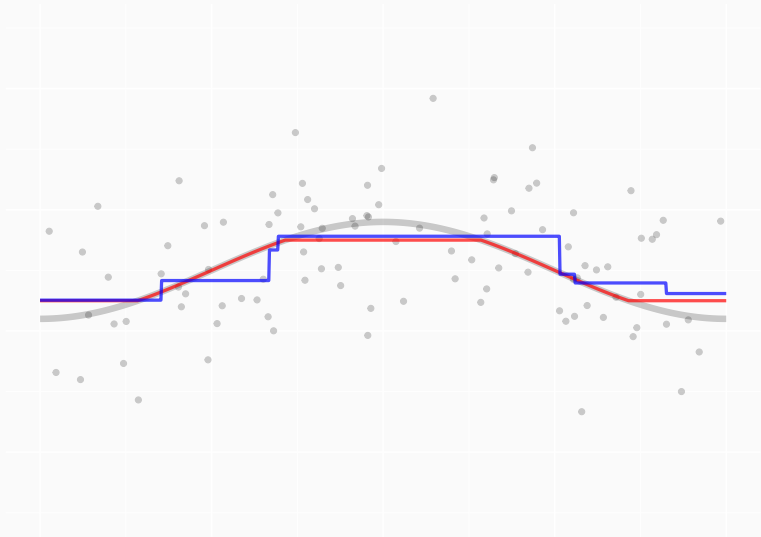


Figure 5: Bounded Variation Curves: $\rho_{TV} \leq 1$ ($n = 100$.)

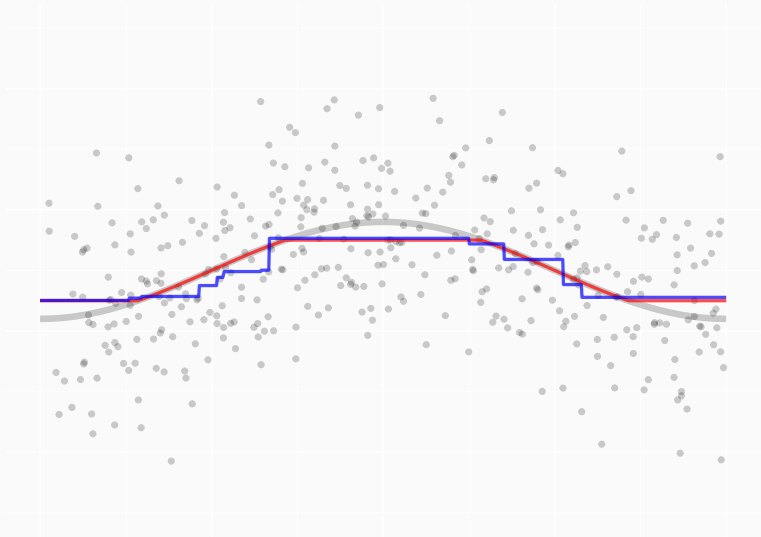


Figure 6: Bounded Variation Curves: $\rho_{TV} \leq 1$. ($n = 400$.)

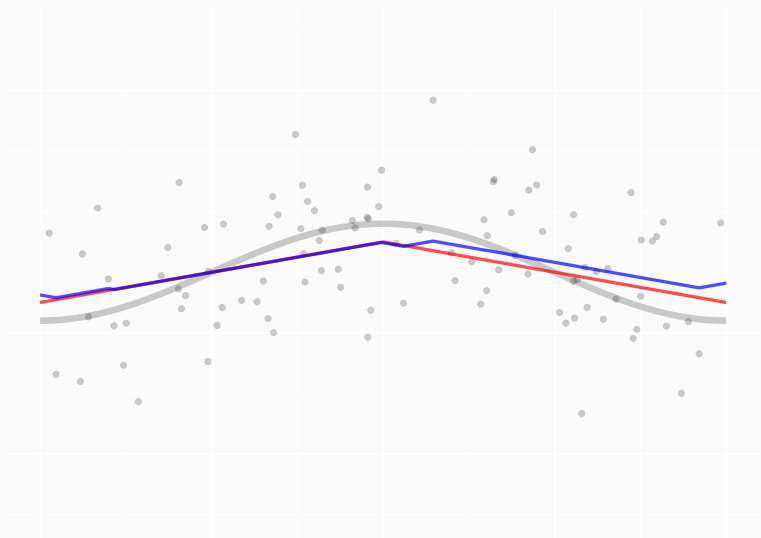


Figure 7: Lipschitz Curves: $\rho_{\text{Lip}} \leq 1$ ($n = 100$.)

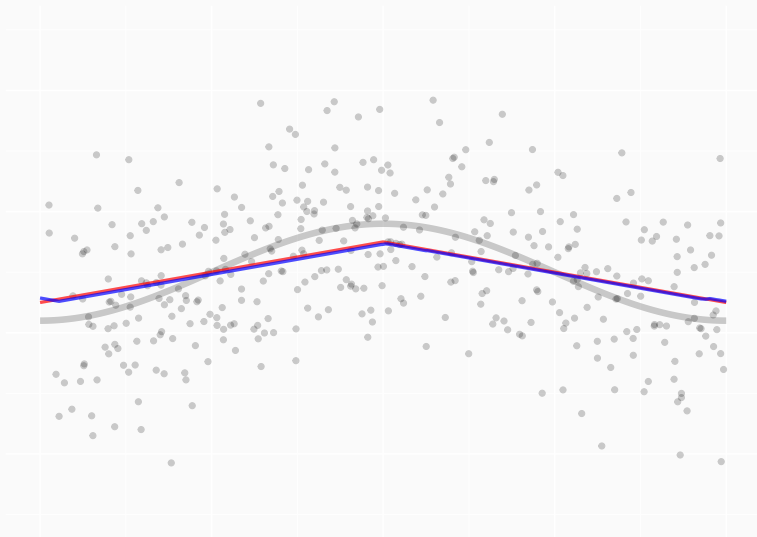


Figure 8: Lipschitz Curves: $\rho_{\text{Lip}} \leq 1$ ($n = 400$.)

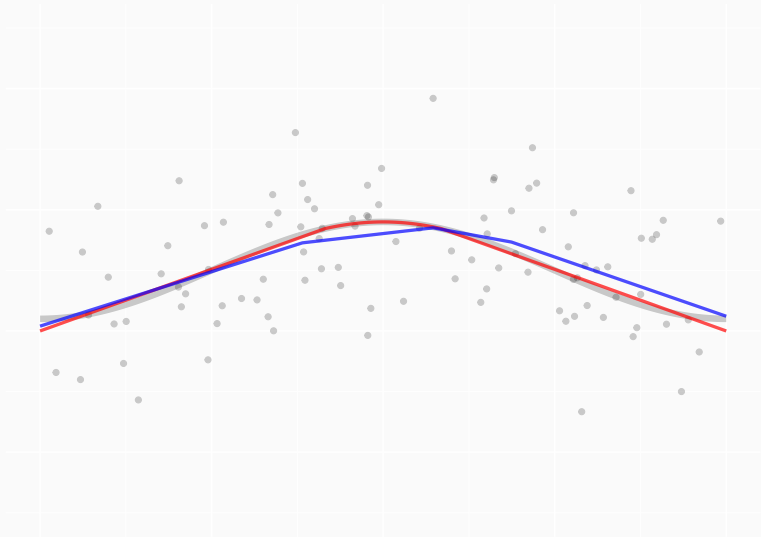


Figure 9: Concave Curves ($n = 100$.)

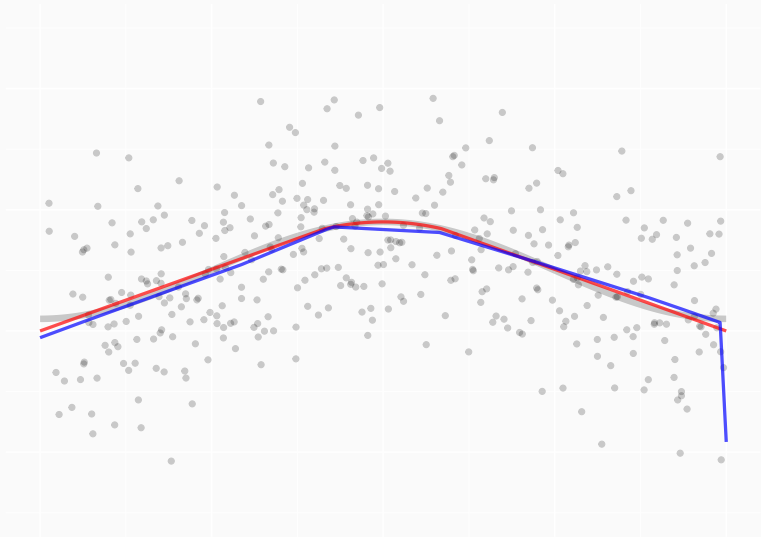


Figure 10: Concave Curves ($n = 400$.)

Non-Gaussian Noise

Starting Point

$$\ell(m) - \ell(\mu^*) = \|m - \mu^*\|_{L_2(P_n)}^2$$

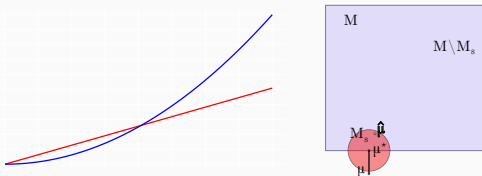
squared distance

$$- \frac{2}{n} \sum_{i=1}^n \varepsilon_i \{m(X_i) - \mu^*(X_i)\}$$

a mean zero term

$$+ \frac{2}{n} \sum_{i=1}^n \{\mu^*(X_i) - \mu(X_i)\} \{m(X_i) - \mu^*(X_i)\}$$

a non-negative term.

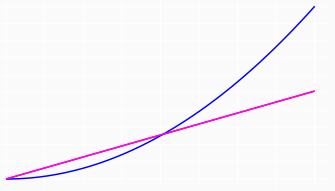


We can bound error using a corresponding *width*, no matter how noise is distributed.

$$\|\hat{\mu} - \mu^*\|_{L_2(P_n)} < s + 2\sqrt{\frac{2\Sigma_n}{\delta n}} \quad \text{w.p. } 1 - \delta \quad \text{for} \quad \frac{s^2}{2} \geq w_\varepsilon(\mathcal{M}_s)$$

$$\text{where } w_\varepsilon(\mathcal{V}) = \mathbb{E} \max_{v \in \mathcal{V}} \langle \varepsilon, v \rangle_{L_2(P_n)} \quad \text{and} \quad \Sigma_n = \mathbb{E} \max_{i \in 1 \dots n} \varepsilon_i^2.$$

This bound depends on the model \mathcal{M} and the distribution of the noise ε in a complex, entangled way: through the width $w_\varepsilon(\mathcal{M}_s)$.



To disentangle the impact of the model and noise distribution, we'll bound this width in terms of gaussian width.

$$w_{\epsilon}(\mathcal{M}_s) \leq \alpha w(\mathcal{M}_s)$$

for α depending on ϵ but not \mathcal{M} or s .

At the heart of this comparison $w_{\epsilon}(\cdot) \leq \alpha w(\cdot)$ are two ideas.

1. **Symmetrization.** We'll substitute for ϵ_i a variant that's symmetric around zero.

$$\epsilon_i \rightarrow \epsilon_i - \epsilon'_i \quad \text{where} \quad \epsilon'_i \text{ is an independent copy of } \epsilon_i$$

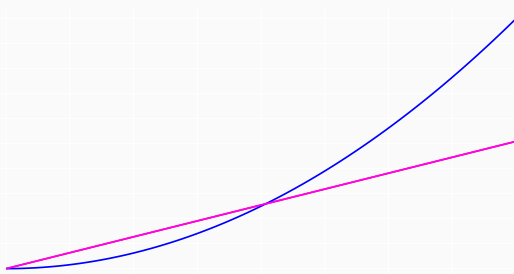
This substitution *increases* width: $w_{\epsilon}(\cdot) \leq w_{\epsilon - \epsilon'}(\cdot)$.

2. **Contraction.** We'll substitute a gaussian vector for our symmetrized noise $\epsilon - \epsilon'$. We can bound the impact of this substitution in a model-invariant way.

$$w_{\epsilon - \epsilon'}(\cdot) \leq \sqrt{2\pi} M_n \times w(\cdot) \quad \text{for} \quad M_n = \mathbb{E} \max_{i \in 1 \dots n} |\epsilon_i|$$

This lets us re-use our gaussian width calculations to analyze regression with any noise distribution.

A Simple Consequence: Width Comparison implies Radius Comparison



- If you have a width comparison $w_\epsilon \leq \alpha w_\eta$ for some $\alpha \geq 1$.
- This implies a radius comparison $s_\epsilon \leq \alpha s_\eta$ for all convex models \mathcal{M} .

$$s_\epsilon = \alpha s_\eta \quad \text{satisfies} \quad \frac{s_\epsilon^2}{2} \geq w_\epsilon(\mathcal{M}_{s_\epsilon}) \quad \text{if} \quad \frac{s_\eta^2}{2} \geq w_\eta(\mathcal{M}_{s_\eta}) \quad \text{for convex } \mathcal{M}$$
$$\text{and} \quad w_\epsilon \leq \alpha w_\eta \quad \text{for} \quad \alpha \geq 1.$$

- *Interpretation.*
The noise ϵ makes regression at most ' α times harder' than the noise η .
- *This is simplistic and 'lossy'.*
For most models, our width comparison implies a better radius comparison.

Proof: Width Comparisons imply Radius Comparisons

Claim. If $w_\varepsilon \leq \alpha w_\eta$ for $\alpha \geq 1$, then for any convex model \mathcal{M} , the critical radius using noise ε is at most α times the critical radius using noise η , i.e.

$$\frac{(\alpha s)^2}{2} \geq w_\varepsilon(\mathcal{M}_{\alpha s}) \quad \text{if} \quad \frac{s^2}{2} \geq w_\eta(\mathcal{M}_s) \quad \text{and} \quad w_\varepsilon \leq \alpha w_\eta \quad \text{for} \quad \alpha \geq 1.$$

Proof. If $s^2/2 \geq w_\eta(\mathcal{M}_s)$, then

Proof: Width Comparisons imply Radius Comparisons

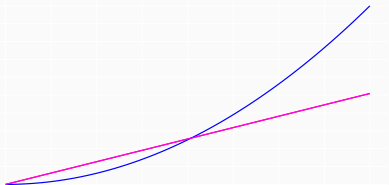
Claim. If $w_\varepsilon \leq \alpha w_\eta$ for $\alpha \geq 1$, then for any convex model \mathcal{M} , the critical radius using noise ε is at most α times the critical radius using noise η , i.e.

$$\frac{(\alpha s)^2}{2} \geq w_\varepsilon(\mathcal{M}_{\alpha s}) \quad \text{if} \quad \frac{s^2}{2} \geq w_\eta(\mathcal{M}_s) \quad \text{and} \quad w_\varepsilon \leq \alpha w_\eta \quad \text{for} \quad \alpha \geq 1.$$

Proof. If $s^2/2 \geq w_\eta(\mathcal{M}_s)$, then

$\alpha s/2 \geq \alpha w_\eta(\mathcal{M}_s)/s$	multiplying both sides by α/s
$\geq \alpha w_\eta(\mathcal{M}_{\alpha s})/(\alpha s)$	using sublinearity of $f(s) = w_\eta(\mathcal{M}_s)$
$\geq w_\varepsilon(\mathcal{M}_{\alpha s})/(\alpha s)$	using our premise $\alpha w_\eta \geq w_\varepsilon$.

Multiplying both sides by αs , we get our claim.



Where we are. We have a bound that depends on the model \mathcal{M} and the distribution of the noise ϵ in a complex and entangled way.

$$\|\hat{\mu} - \mu^*\|_{L_2(\mathcal{P}_n)} < s_\epsilon + 2\sqrt{\frac{2\Sigma_n}{\delta n}} \quad \text{w.p. } 1 - \delta \quad \text{for} \quad \frac{s_\epsilon^2}{2} \geq w_\epsilon(\mathcal{M}_{s_\epsilon})$$

$$\text{where } w_\epsilon(\mathcal{V}) = \mathbb{E} \max_{v \in \mathcal{V}} \langle \epsilon, v \rangle_{L_2(\mathcal{P}_n)} \quad \text{and} \quad \Sigma_n = \mathbb{E} \max_{i \in 1 \dots n} \epsilon_i^2.$$

Where we're going. We'll derive a bound that depends on the model \mathcal{M} and the distribution of the noise ϵ in simpler and disentangled way.

$$\|\hat{\mu} - \mu^*\|_{L_2(\mathcal{P}_n)} < \sqrt{2\pi} M_n s + 2\sqrt{\frac{2\Sigma_n}{\delta n}} \leq \quad \text{w.p. } 1 - \delta \quad \text{for} \quad \frac{s^2}{2} \geq w(\mathcal{M}_s)$$

$$\text{where } w(\mathcal{V}) = \mathbb{E} \max_{v \in \mathcal{V}} \langle g, v \rangle_{L_2(\mathcal{P}_n)} \quad \text{and} \quad M_n = \mathbb{E} \max_{i \in 1 \dots n} |\epsilon_i|.$$

Better yet. We can simplify it into a bound that depends on only one measure of noise complexity.

$$\|\hat{\mu} - \mu^*\|_{L_2(\mathcal{P}_n)} \leq \sqrt{2\pi\Sigma_n} \left(s + \sqrt{\frac{2}{\delta n}} \right) \quad \text{because} \quad M_n \leq \sqrt{\Sigma_n} \quad \text{and} \quad 2 \leq \sqrt{2\pi}$$

Non-Gaussian Noise

Example: Probabilistic Classification

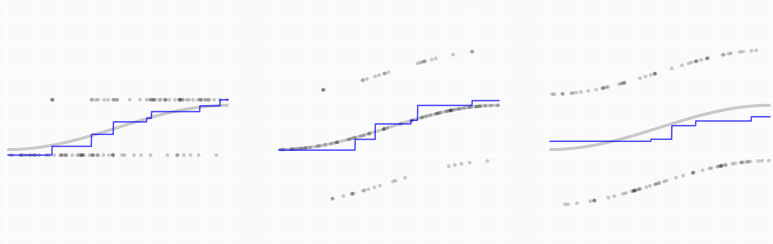


Figure 11: classification noise \rightarrow symmetrized classification noise \rightarrow random-sign noise

Suppose we have independent *binary observations*.

$$\begin{aligned} Y_i &= \begin{cases} 1 & \text{with conditional probability } \mu(X_i) \\ 0 & \text{otherwise} \end{cases} \\ &= \mu(X_i) + \varepsilon_i \quad \text{for} \quad \varepsilon_i = \begin{cases} 1 - \mu(X_i) & \text{with conditional probability } \mu(X_i) \\ -\mu(X_i) & \text{with conditional probability } 1 - \mu(X_i) \end{cases}. \end{aligned}$$

Note that this *classification noise* ε_i has conditional mean zero.

$$\mathbb{E}[\varepsilon_i \mid X_i] = \mu(X_i)\{1 - \mu(X_i)\} + \{1 - \mu(X_i)\}\{-\mu(X_i)\} = 0.$$

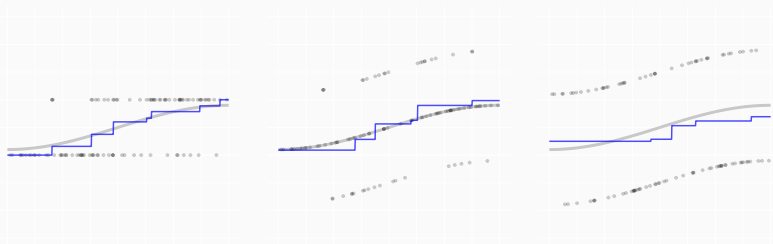


Figure 11: classification noise \rightarrow symmetrized classification noise \rightarrow random-sign noise

What we need to bound is *classification-noise width*

$$w_{\epsilon}(\mathcal{V}) = \frac{1}{n} \mathbb{E} \max_{v \in \mathcal{V}} \sum_{i=1}^n \epsilon_i v_i.$$

We'll show it's no bigger than a version with *symmetrized noise*.

$$\epsilon_i - \epsilon'_i = \begin{cases} +1 & \text{when } \epsilon_i = 1 - \mu(X_i), \epsilon'_i = \mu(X_i) \\ -1 & \text{when } \epsilon_i = \mu(X_i), \epsilon'_i = 1 - \mu(X_i) \\ 0 & \text{when } \epsilon_i = \epsilon'_i \end{cases}$$

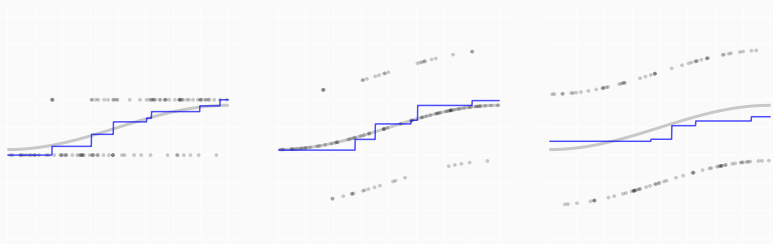


Figure 11: classification noise \rightarrow symmetrized classification noise \rightarrow random-sign noise

And we'll show that *this* is no bigger than a version with *random sign noise*

$$w_{\epsilon}(\mathcal{V}) \leq w_{\epsilon-\epsilon'}(\mathcal{V}) \leq w_s(\mathcal{V}) \quad \text{where} \quad s_i = \pm 1 \text{ w.p. } 1/2.$$

The trick will be multiplying the symmetrized noise by a random sign.

It's already symmetric, so that doesn't change its distribution.

$$\epsilon_i - \epsilon'_i \stackrel{\text{dist}}{=} s_i(\epsilon_i - \epsilon'_i)$$

Then we'll *contract out* the symmetrized noise, leaving the random sign. You'll see.

Step 1

We bound our maximum in terms of one involving symmetric noise.

We'll work with an *independent copy* ε' of our noise vector ε .

$$\begin{aligned} \mathbb{E}_{\varepsilon} \max_{v \in \mathcal{V}} \sum_{i=1}^n \varepsilon_i v_i &\stackrel{(a)}{=} \mathbb{E}_{\varepsilon} \max_{v \in \mathcal{V}} \sum_{i=1}^n (\varepsilon_i - \mathbb{E}_{\varepsilon'} \varepsilon'_i) v_i \\ &\stackrel{(b)}{=} \mathbb{E}_{\varepsilon} \max_{v \in \mathcal{V}} \mathbb{E}_{\varepsilon'} \sum_{i=1}^n (\varepsilon_i - \varepsilon'_i) v_i \\ &\stackrel{(c)}{\leq} \mathbb{E}_{\varepsilon} \mathbb{E}_{\varepsilon'} \max_{v \in \mathcal{V}} \sum_{i=1}^n (\varepsilon_i - \varepsilon'_i) v_i. \end{aligned}$$

Why do these steps work?

(a) $\mathbb{E}_{\varepsilon'} \varepsilon'_i = 0$.

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Why do these steps work?

- (a) $\mathbb{E}_{\varepsilon'} \varepsilon'_i = 0$.
- (b) Expectation is linear.
- (c) Maximizing the average gives us something smaller than averaging the maxima.

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- (a) $\mathbb{E}_{\varepsilon'} \varepsilon'_i = 0$.
- (b) Expectation is linear.
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 - In (c), we choose the maximizing $v \in \mathcal{V}$ for each ε' .

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Why do these steps work?

- (a) $\mathbb{E}_{\varepsilon'} \varepsilon'_i = 0$.
- (b) Expectation is linear.
- (c) Maximizing the average gives us something smaller than averaging the maxima.
 - In (c), we choose the maximizing $v \in \mathcal{V}$ for each ε' .
 - If we wanted to choose the same one each time, like we do in (b), we could.

We introduce independent random signs $s_i = \pm 1$ w.p. $1/2$, changing nothing.

$$\mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} \max_{v \in \mathcal{V}} \sum_{i=1}^n (\varepsilon_i - \varepsilon'_i) v_i = \mathbb{E}_s \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i.$$

Why does this change nothing?

We introduce independent random signs $s_i = \pm 1$ w.p. $1/2$, changing nothing.

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Why does this change nothing?

- Because the inner mean $(\mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'})$ doesn't depend on the signs s_i .
- That's because ε_i and ε'_i have the same distribution.
- And this implies $(\varepsilon_i - \varepsilon'_i)$ and $(\varepsilon'_i - \varepsilon) = -(\varepsilon_i - \varepsilon'_i)$ do, too.

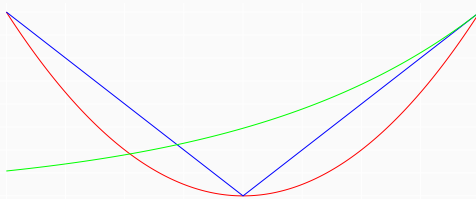
Step 3

We swap the order of our averages and think about the inner average as a *function* of our vector of symmetric noise.

$$\begin{aligned} \mathbb{E}_s \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i &= \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i \\ &= \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} f(\varepsilon - \varepsilon') \quad \text{for} \quad f(u) = \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i u_i v_i. \end{aligned}$$

This function f is convex.

What does that mean? These, for example, are all convex.



$$f\{(1-\lambda)a + \lambda b\} \leq (1-\lambda)f(a) + \lambda f(b) \quad \text{for} \quad \lambda \in [0, 1]. \quad \text{That's Convexity}$$

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This function f is convex.

How do we know? Maximizing each term is better than maximizing their sum.

$$\begin{aligned} f\{(1-\lambda)a + \lambda b\} &= \mathbb{E}_s \max_{v \in \mathcal{V}} \left\{ (1-\lambda) \sum_{i=1}^n s_i a_i v_i + \lambda \sum_{i=1}^n s_i b_i v_i \right\} \\ &\leq \mathbb{E}_s \left\{ \max_{v \in \mathcal{V}} (1-\lambda) \sum_{i=1}^n s_i a_i v_i + \max_{v \in \mathcal{V}} \lambda \sum_{i=1}^n s_i b_i v_i \right\} \\ &= (1-\lambda) \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i a_i v_i + \lambda \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i b_i v_i \\ &= (1-\lambda)f(a) + \lambda f(b). \end{aligned}$$

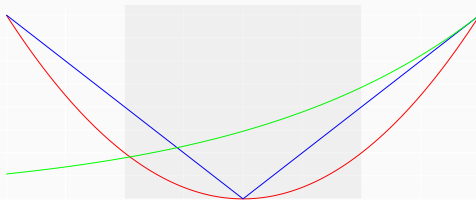
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$$\begin{aligned} \mathbb{E}_s \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i &= \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i \\ &= \mathbb{E}_\varepsilon \mathbb{E}_{\varepsilon'} f(\varepsilon - \varepsilon') \quad \text{for} \quad f(u) = \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i u_i v_i. \end{aligned}$$

This function f is convex.

Why does this matter? The max of a convex function over a cube occurs at a corner.



What cube?

The vector of symmetric noise, $\varepsilon - \varepsilon'$, is in the *unit cube* $[-1, 1]^n$.

$$\varepsilon_i - \varepsilon'_i = \begin{cases} 0 & \text{when } \varepsilon_i = \varepsilon'_i \\ +1 & \text{when } \varepsilon_i = 1 - \mu(X_i), \varepsilon'_i = \mu(X_i) \\ -1 & \text{when } \varepsilon_i = \mu(X_i), \varepsilon'_i = 1 - \mu(X_i). \end{cases}$$

The average over this random vector is bounded by the maximum over the cube it's in.

$$\begin{aligned} \mathbb{E}_{\varepsilon} \mathbb{E}_{\varepsilon'} \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i &\leq \max_{u \in [-1, 1]^n} \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i u_i v_i \\ &= \max_{u \in [-1, 1]^n} f(u) \quad \text{max over the cube} \\ &= \max_{u \in \{-1, 1\}^n} f(u) \quad \text{max over its corners} \end{aligned}$$

We characterize this maximum over corners. Remember what f is.

$$\begin{aligned}\max_{u \in \{-1,1\}^n} f(u) &= \max_{u \in \{-1,1\}^n} \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i u_i v_i \\ &= \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i v_i.\end{aligned}$$

Why?

Hint. What's the distribution of s_i ? And $s_i u_i$ for $u_i \in \{-1,1\}$?

We characterize this maximum over corners. Remember what f is.

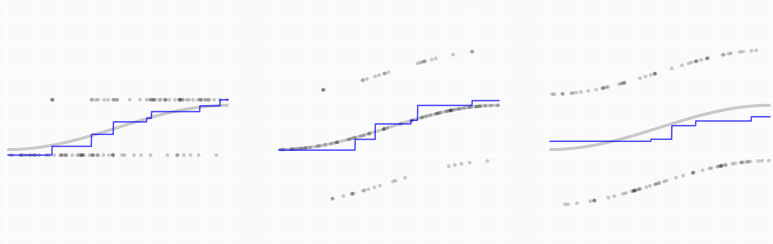
$$\begin{aligned}\max_{u \in \{-1, 1\}^n} f(u) &= \max_{u \in \{-1, 1\}^n} \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i u_i v_i \\ &= \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i v_i.\end{aligned}$$

Why?

Hint. What's the distribution of s_i ? And $s_i u_i$ for $u_i \in \{-1, 1\}$?

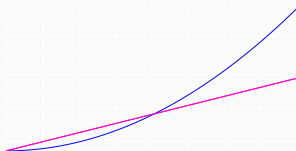
- For $u_i \in \{-1, 1\}$, the distributions of u_i and $s_i u_i$ are the same.
- So the distribution of the sum, and its maximum, are the same at every corner u .
- Including the vector of all ones $u = (1, 1, \dots, 1)$.

Summary



classification noise width \leq symmetrized classification noise width \leq random sign width
 This means probabilistic classification is *easier* than regression with random sign noise. Or, at least, that we get a better bound.

$$\frac{s^2}{2} \geq w_s(\mathcal{M}_s) \quad \text{and} \quad w_s(\mathcal{M}_s) \geq w_\varepsilon(\mathcal{M}_s) \quad \implies \quad \frac{s^2}{2} \geq w_\varepsilon(\mathcal{M}_s)$$



People call random sign width, or something like it, *Rademacher Complexity*.

$$\text{Rademacher Complexity}(\mathcal{V}) = \mathbb{E} \max_{v \in \mathcal{V}} \langle s, v \rangle_{L_2(\mathbf{P}_n)} \quad \text{for i.i.d. } s_i = \begin{cases} +1 & \text{w.p. } 1/2 \\ -1 & \text{w.p. } 1/2 \end{cases}$$

or maybe $= \mathbb{E} \max_{v \in \mathcal{V}} |\langle s, v \rangle_{L_2(\mathbf{P}_n)}|$

- This second definition is the same if \mathcal{V} is symmetric, i.e. $v \in \mathcal{V} \implies -v \in \mathcal{V}$.
- Otherwise, it can be a little bigger.
 - At most $2\times$ bigger. Prove it!
 - Use the bound $\max a, b \leq a + b$ and the symmetry of s 's distribution.

Non-Gaussian Noise

The General Case

Symmetrization and Contraction: Examples

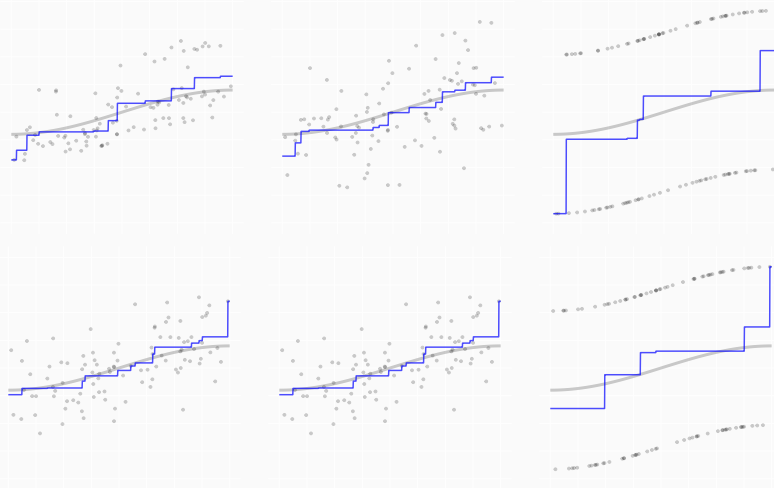


Figure 12: real noise \rightarrow symmetrized noise \rightarrow scaled sign noise

$$w_{\varepsilon}(\mathcal{V}) \leq w_{s(\varepsilon - \varepsilon')}(\mathcal{V}) \leq 2 w_{s\varepsilon}(\mathcal{V})$$

$$\begin{aligned} \mathbb{E} \max_{v \in \mathcal{V}} \sum_{i=1}^n \varepsilon_i v_i &= \mathbb{E} \max_{v \in \mathcal{V}} \sum_{i=1}^n (\varepsilon_i - \mathbb{E} \varepsilon'_i) v_i \\ &\stackrel{(a)}{\leq} \mathbb{E} \mathbb{E}' \max_{v \in \mathcal{V}} \sum_{i=1}^n (\varepsilon_i - \varepsilon'_i) v_i \\ &= \mathbb{E}_s \mathbb{E} \mathbb{E}' \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i (\varepsilon_i - \varepsilon'_i) v_i \\ &\stackrel{(b)}{\leq} \mathbb{E}_s \mathbb{E} \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i \varepsilon_i + \mathbb{E}_s \mathbb{E}' \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i \varepsilon'_i v_i \\ &= 2 \mathbb{E}_s \mathbb{E} \max_{v \in \mathcal{V}} \sum_{i=1}^n \varepsilon_i s_i v_i. \end{aligned}$$

(a) Replacing ε_i with $s_i(\varepsilon_i - \varepsilon'_i)$ is 'free'.

- We stopped here in our example because $\varepsilon_i - \varepsilon'_i$ was easy to bound.
- Generally, we take an extra step to express things in terms of ε_i again.

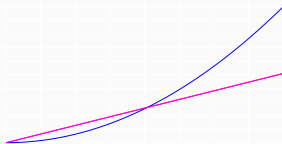
(b) Replacing ε_i with $s_i \varepsilon_i$ increases width by at most $2 \times$.

$$w_\eta(\mathcal{V}) = w_{s\eta}(\mathcal{V}) \leq E\|\eta\|_\infty w_\eta(\mathcal{V}) \quad \text{if } \eta \stackrel{\text{dist}}{=} -\eta.$$

$$\begin{aligned} E_s E_\eta \max_{v \in \mathcal{V}} \sum_{i=1}^n \eta_i s_i v_i &\leq E_\eta \max_{\substack{u \in \mathbb{R}^n \\ \|u_i\| \leq \|\eta\|_\infty}} E_s \max_{v \in \mathcal{V}} \sum_{i=1}^n u_i s_i v_i \\ &= E_\eta \|\eta\|_\infty \max_{u \in [-1, 1]^n} E_s \max_{v \in \mathcal{V}} \sum_{i=1}^n u_i s_i v_i \\ &= E_\eta \|\eta\|_\infty \times \max_{u \in [-1, 1]^n} E_s \max_{v \in \mathcal{V}} \sum_{i=1}^n u_i s_i v_i \\ &= E_\eta \|\eta\|_\infty \times E_s \max_{v \in \mathcal{V}} \sum_{i=1}^n s_i v_i \end{aligned}$$

- We can 'contract out' any **symmetrically distributed** noise vector η by ...
 1. multiplying in independent random signs s_i . Symmetry $\implies s_i \eta_i \stackrel{\text{dist}}{=} \eta_i$.
 2. maximizing over a cube containing η .
- We just have to use a big enough cube.
 - In our example, $\eta = \varepsilon - \varepsilon'$ was in the unit cube $[-1, 1]^n$ deterministically.
 - Generally, we maximize over a random cube $[-\|\eta\|_\infty, \|\eta\|_\infty]^n$.
 - And we can pull out the cube's radius $\|\eta\|_\infty$ as a multiplicative factor.

Implications for Regression



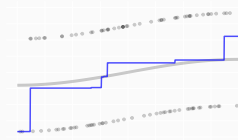
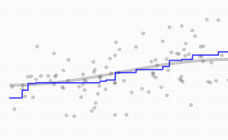
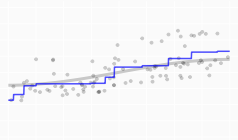
$$w_{\varepsilon}(\mathcal{V}) \leq \mathbb{E} \|\varepsilon_i - \varepsilon'_i\|_{\infty} w_s(\mathcal{V}) \leq 2 \mathbb{E} \|\varepsilon_i\|_{\infty} w_s(\mathcal{V})$$

Regression with arbitrary independent noise, i.e.

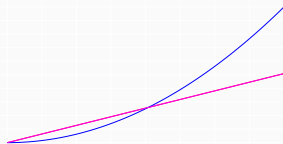
$$Y_i = \mu(X_i) + \varepsilon_i \quad \text{where} \quad \varepsilon_1 \dots \varepsilon_n \text{ are independent,}$$

is no harder than with scaled-up random sign noise, i.e.

$$Y_i = \mu(X_i) + M s_i \quad \text{for} \quad M = \mathbb{E} \|\varepsilon_i - \varepsilon'_i\|_{\infty} \quad \text{and} \quad s_i = \begin{cases} +1 & \text{w.p. } 1/2 \\ -1 & \text{w.p. } 1/2 \end{cases}.$$



The Symmetric Case



$$w_\varepsilon(\mathcal{V}) \leq \mathbb{E}\|\varepsilon_i\|_\infty w_s(\mathcal{V})$$

Regression with arbitrary independent *symmetric* noise, i.e.

$$Y_i = \mu(X_i) + \varepsilon_i \quad \text{where} \quad \varepsilon_1 \dots \varepsilon_n \text{ are independent with } \varepsilon_i \stackrel{\text{dist}}{=} -\varepsilon_i,$$

is no harder than with scaled-up random sign noise, i.e.

$$Y_i = \mu(X_i) + Ms_i \quad \text{for}^2 \quad M = \mathbb{E}\|\varepsilon_i\|_\infty \quad \text{and} \quad s_i = \begin{cases} +1 & \text{w.p. } 1/2 \\ -1 & \text{w.p. } 1/2 \end{cases}.$$

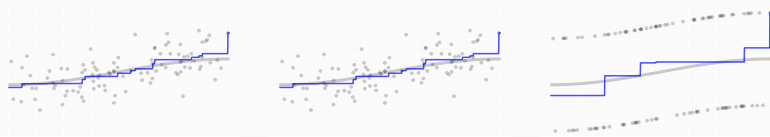
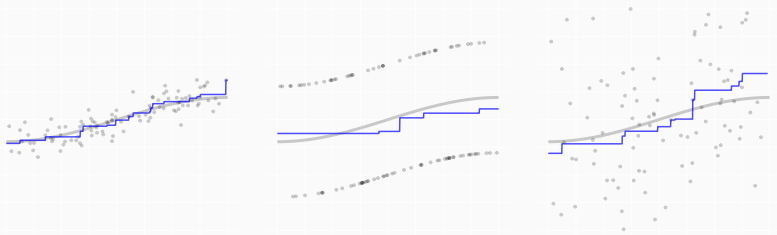


Figure 13: real noise \rightarrow symmetrized noise \rightarrow scaled sign noise

² $M = \mathbb{E}\|\varepsilon_i\|_\infty \leq 2\sigma\sqrt{2\log(2n)}$ for $\varepsilon_i \sim N(0, \sigma^2)$. See Appendix B of the Gaussian Width Homework.

Non-Gaussian Noise

Comparison to the Gaussian Case



- So far, we've bounded arbitrary-noise width in terms of random-sign width.
- But often, it's easier to understand gaussian width. That's good enough.³

$$\frac{1}{2\sqrt{\log(2n)}} w_g(\mathcal{V}) \leq w_s(\mathcal{V}) \leq \sqrt{\frac{\pi}{2}} w_g(\mathcal{V})$$

$\approx .2 \text{ for } n=100$ ≈ 1.25

- We just saw it can't be **that much bigger** than random-sign width.
- And we can show it's **at least 4/5 as big**.

$$\mathbb{E} \max_{v \in \mathcal{V}} \sum_{i=1}^n g_i v_i = \mathbb{E}_s \mathbb{E}_g \max_{v \in \mathcal{V}} \sum_{i=1}^n |g_i| s_i v_i \geq \mathbb{E}_s \max_{v \in \mathcal{V}} \sum_{i=1}^n \mathbb{E}_g |g_i| s_i v_i = \sqrt{\frac{2}{\pi}}$$

³We can show $.125 w_g(\mathcal{V}) \leq w_s(\mathcal{V}) \leq 1.25 w_g(\mathcal{V})$ for $n \leq 10$ trillion by bounding $\mathbb{E} \|g\|_\infty$ more carefully.

Comparison in Steps

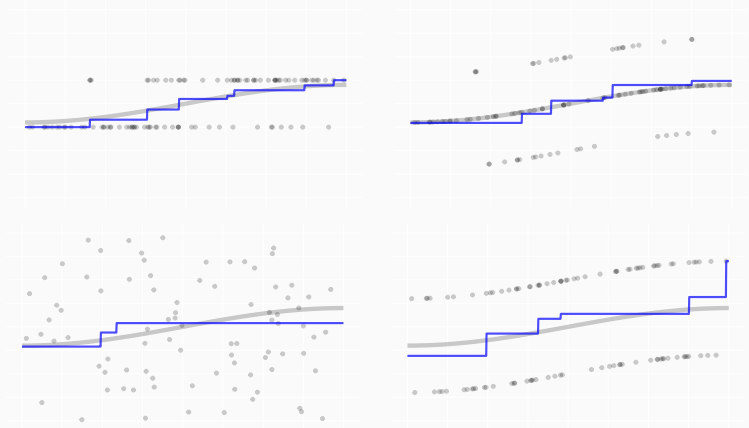


Figure 14: real noise \rightarrow symmetrized noise \downarrow scaled sign noise \leftarrow scaled gaussian noise

$$w_{\varepsilon}(\mathcal{V}) \leq w_{\varepsilon - \varepsilon'}(\mathcal{V}) \leq \underset{\leq 2 \mathbb{E} \|\varepsilon\|_{\infty}}{\mathbb{E} \|\varepsilon - \varepsilon'\|_{\infty}} \quad w_s(\mathcal{V}) \leq \sqrt{\frac{\pi}{2}} \mathbb{E} \|\varepsilon - \varepsilon'\|_{\infty} \quad w_g(\mathcal{V}) \leq \sqrt{2\pi} \approx 2.5 \times \mathbb{E} \|\varepsilon\|_{\infty}$$

Implications for Regression

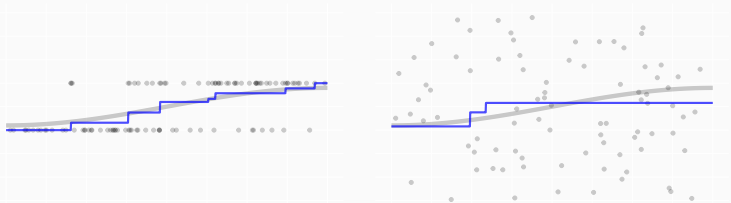


Figure 15: real noise \rightarrow scaled gaussian noise

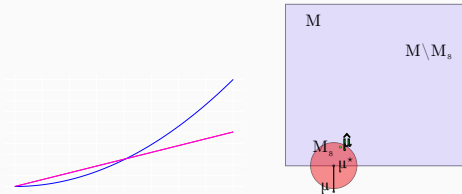
For any noise vector ε with independent components ε_i ,

$$w_{\varepsilon}(\mathcal{V}) \leq 2 \mathbb{E} \|\varepsilon\|_{\infty} \cdot w_s(\mathcal{V}) \leq \sqrt{2\pi} \mathbb{E} \|\varepsilon\|_{\infty} \cdot w_g(\mathcal{V}).$$

- We can bound the width w_{ε} in terms of
 1. random-sign width
 2. the maximum absolute value of ε 's components.
- And we can bound random-sign width in terms of gaussian width.

This means we don't have to bound a million different kinds of widths for each model.
We can bound random-sign width or gaussian width. Whichever is easier.

Sampling



We have a bound that's valid for any signal μ and any vector of independent noise ε .

$$\|\hat{\mu} - \mu^*\|_{L_2(\mathcal{P}_n)} < \sqrt{2\pi\Sigma_n} \left(s + \sqrt{\frac{2}{\delta n}} \right) \quad \text{w.p. } 1 - \delta$$

- It depends on the model's size through the *critical radius*.

s satisfying $s^2/2 \geq \mathbf{w}(\mathcal{M}_s)$ for $\mathcal{M}_s = \{m \in \mathcal{M} : \|m - \mu^*\|_{L_2(\mathcal{P}_n)} \leq s\}$

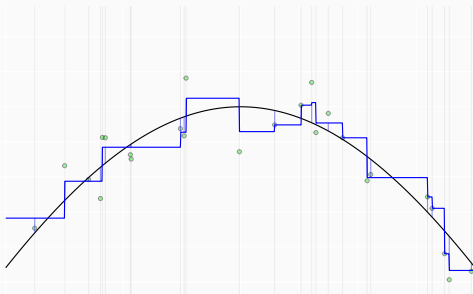
- This is a one-number summary of the gaussian width of neighborhoods ...
- ...of the model's best approximation to the signal. It's the summary that matters.
- It depends on the noise's size through the expected maximum square.

$$\Sigma_n = \mathbb{E} \max_{i \in 1 \dots n} |\varepsilon_i|^2$$

What does this tell us?

Bounds like this say how close $\hat{\mu}$ and μ^* are, on average, on our sample $X_1 \dots X_n$.

$$\frac{1}{n} \sum_{i=1}^n \{\hat{\mu}(X_i) - \mu^*(X_i)\} < \dots$$



It doesn't tell us how close they are in the gaps between those points.

- Let's think about what happens when $X_1 \dots X_n$ are drawn independently from some distribution \mathbf{P} . Think sampling with replacement from a population.
- We'll bound the *population root mean squared error* $\|\hat{\mu} - \mu^*\|_{L_2(\mathbf{P})}$.

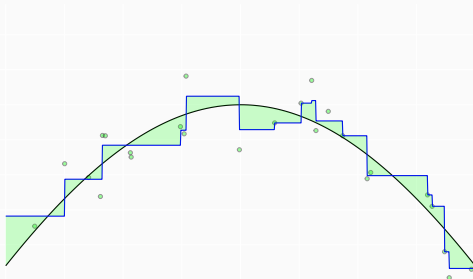
What Population Mean Squared Error Is

It's the mean squared error we make at random point X' distributed like $X_1 \dots X_n$.

$$\|\hat{\mu} - \mu^*\|_{L_2(\mathbf{P})}^2 = \mathbb{E}_{X'} [\{\hat{\mu}(X') - \mu^*(X')\}^2]$$

That's the integral of the squared distance between the two curves,
multiplied by the density of X_i .

$$\|\hat{\mu} - \mu^*\|_{L_2(\mathbf{P})}^2 = \int \{\hat{\mu}(x) - \mu^*(x)\}^2 p(x) dx \quad \text{if } X_i \text{ has the density } p(x).$$

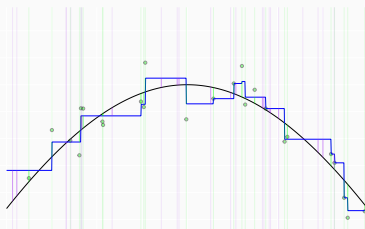


Why we care about Population Mean Squared Error: Generalization

If we're interested in average accuracy for a bunch of new points $X'_1 \dots X'_{n'}$, distributed like $X_1 \dots X_n$, that's more or less exactly what it is.

$$\|\hat{\mu} - \mu\|_{L_2(P)}^2 = E_{X'} [\{\hat{\mu}(X') - \mu(X')\}^2] \stackrel{LLN}{\approx} \frac{1}{n'} \sum_{i=1}^{n'} \{\hat{\mu}(X'_i) - \mu(X'_i)\}^2.$$

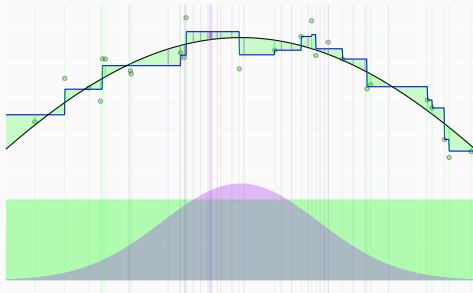
This can be a bit different from accuracy on our original sample $X_1 \dots X_n$.



- BV regression spends its 'variation budget' jumping to fit on the original sample.
- Between those points, it doesn't know whether it should jump or not.
 - So we can get larger error at our new points.
 - It's usually not much larger, but sometimes it is. We'll see why.

Why we care about Population Mean Squared Error: Generalization

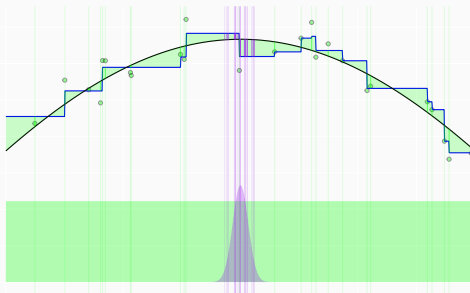
If we're interested in average accuracy for new points from a different distribution Q , we can bound this by comparing this distribution's density to that of our observations.



$$\begin{aligned} \frac{1}{n'} \sum_{i=1}^{n'} \{\hat{\mu}(X'_i) - \mu(X'_i)\}^2 &\approx \|\hat{\mu} - \mu\|_{L_2(Q)}^2 = \int \{\hat{\mu}(x) - \mu(x)\}^2 \frac{q(x)}{p(x)} p(x) dx \\ &\leq \max_x \frac{q(x)}{p(x)} \|\hat{\mu} - \mu\|_{L_2(P)}^2. \end{aligned}$$

Why we care about Population Mean Squared Error: Generalization

If we're interested in accuracy at a specific point x' , we can think of this new distribution Q as a little bump around x' .



$$\{\hat{\mu}(x') - \mu(x')\}^2 \approx \|\hat{\mu} - \mu\|_{L_2(Q_\epsilon)}^2 \quad \text{for} \quad Q = N(x', \epsilon^2).$$

What Does Our Bound Tell Us About This?

Idea. Suppose we know that $\hat{\mu}$ is in a neighborhood \mathcal{M}_s of μ^* . We can ...

- (a) Bound the expected maximum difference between population and sample mean squared error for curves in \mathcal{M}_s .
- (b) Write population mean squared error as an expectation over an independent copy of our sample.
- (c) Compare the result to a maximum of an average of symmetric random variables.

$$\begin{aligned} \mathbb{E} [\|\hat{\mu} - \mu^*\|_{L_2(P)} - \|\hat{\mu} - \mu^*\|_{L_2(P_n)}] &\stackrel{(a)}{\leq} \mathbb{E} \max_{\delta \in \mathcal{M}_s - \mu^*} |\|\delta\|_{L_2(P)} - \|\delta\|_{L_2(P_n)}| \\ &\stackrel{(b)}{=} \mathbb{E}_X \max_{\delta \in \mathcal{M}_s - \mu^*} \mathbb{E}_{X'} \frac{1}{n} \sum_{i=1}^n \delta(X'_i)^2 - \frac{1}{n} \sum_{i=1}^n \delta(X_i)^2 \\ &\stackrel{(c)}{\leq} \mathbb{E}_X \mathbb{E}_{X'} \max_{\delta \in \mathcal{M}_s - \mu^*} \frac{1}{n} \sum_{i=1}^n \delta(X'_i)^2 - \delta(X_i)^2 \end{aligned}$$

Now, in the spirit of our noise comparisons, we can try to compare this to something we know: the random sign width of \mathcal{M}_s . How does ...

$$\dots = \mathbb{E}_X \mathbb{E}_{X'} \mathbb{E}_s \max_{\delta} \frac{1}{n} \sum_{i=1}^n s_i \{\delta(X'_i)^2 - \delta(X_i)^2\}$$

Claim. If ψ is a function with $\psi(0) = 0$ and $\rho_{\text{Lip}}(\psi) \leq L$, then

$$\mathbb{E}_s \max_f \sum_{i=1}^n s_i \psi_i \{f(X'_i)\}^2 \leq L \max_f \sum_{i=1}^n s_i \delta(X_i)^2$$

Consequence. Letting $\psi(x) = x^2$,

$$\mathbb{E}_s \max_{\delta} \sum_{i=1}^n s_i \delta(X_i)^2 \leq L \max_{\delta} \sum_{i=1}^n s_i \delta(X_i) \quad \text{for} \quad L = \max_i |\psi' \{\delta(X_i)\}| = 2\|\delta\|_{L_{\infty}(\mathbb{P}_n)}.$$

i.e.

$$\mathbb{E}_s \max_{\delta} \frac{1}{n} \sum_{i=1}^n s_i \delta(X_i)^2 \leq 2\|\delta\|_{L_{\infty}(\mathbb{P}_n)} w(\mathcal{M}_s)$$

Clever about it the infinity norm. 1. Bake in the constraint. 2. Bounded data — argue that you won't go above or below [e.g. monotone or lipschitz] 3. Suppose we know $\hat{\mu}$ crosses μ somewhere on $[0, 1]$. Then a derivative bound implies an infinity norm bound.