Machine Learning Theory

Lecture 9: Multivariate Regression and the Curse of Dimensionality

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Emory University

Today

1. Sobolev Models Review
2. Homework Review
   - Gaussian Width Calculations
   - Error Bounds for Sobolev Regression
3. Multidimensional Sobolev Models and the Curve of Dimensionality

Sobolev Models Review

The Model

A Sobolev model is the set of curves satisfying a bound on a derivative's mean square.

$$\mathcal{M}^p = \left\{ m \;\; : \;\; \left\| \frac{d^p}{dx^p} m \right\|_{L_2}^2 \le B^2 \right\}$$

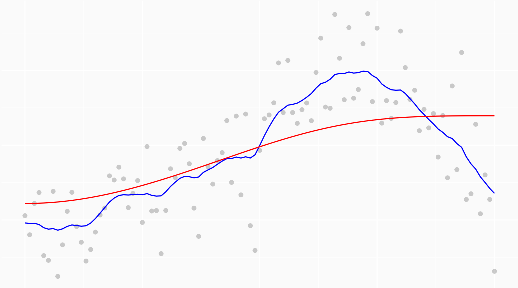

Figure 1: Least squares estimators for p=1 and p=2

They have an equivalent characterization as combinations of orthonormal *cosine basis functions* with coefficients in an ellipse.

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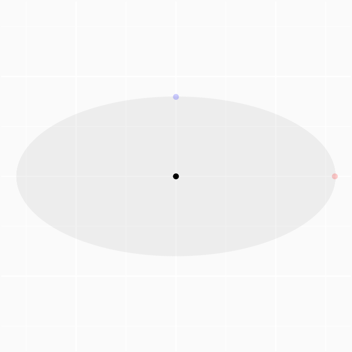

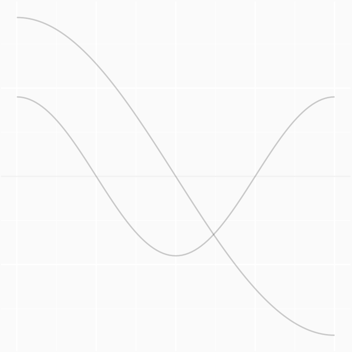

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Fourier Series

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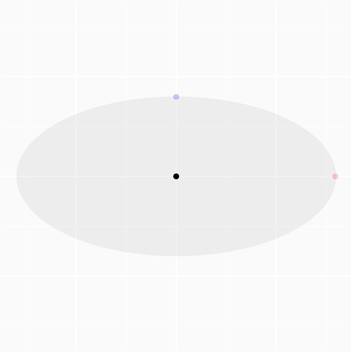

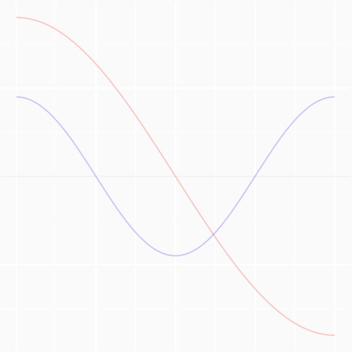

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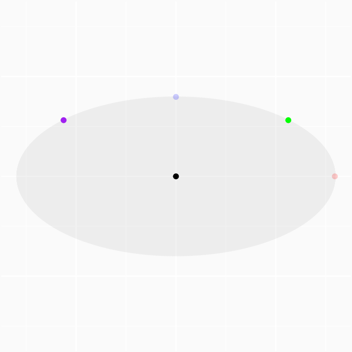

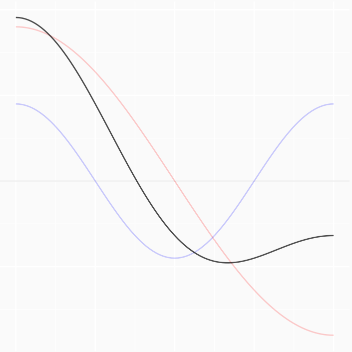

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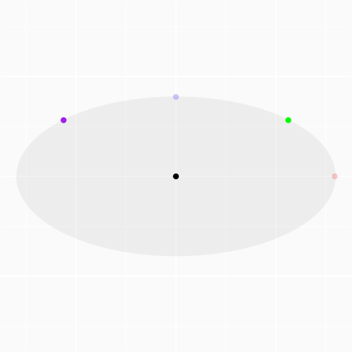

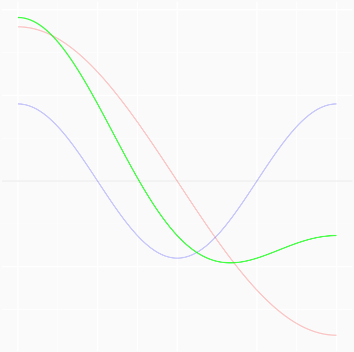

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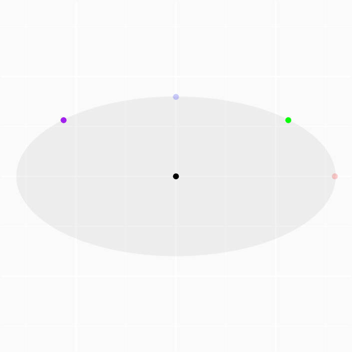

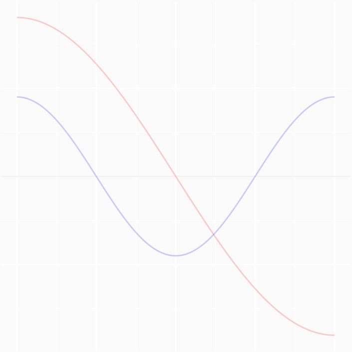

Exercise. Draw the curve with the purple coefficients.

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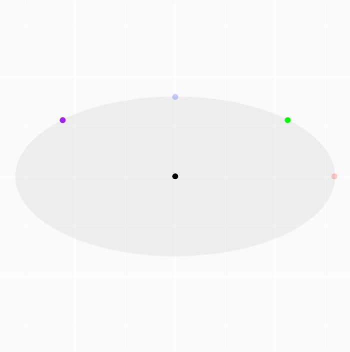

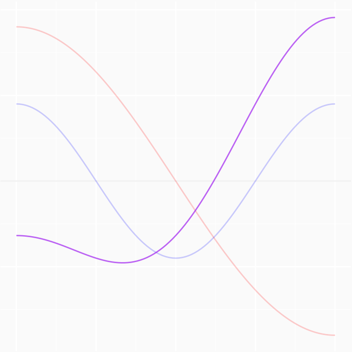

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Sobolev Models Review

How we know this

A useful characterization

We use integration by parts to write our model in terms of *a self-adjoint operator* on the vector space of even 2-periodic functions: the negated second derivative.

$$\mathcal{M}^1 = \left\{ m \;\; : \;\; \left\| \frac{d}{dx} m \right\|_{L_2}^2 \leq B^2 \right\} = \left\{ m \;\; : \;\; \left\langle -\frac{d^2}{dx^2} m, \; m \right\rangle_{L_2} \leq B^2 \right\}$$

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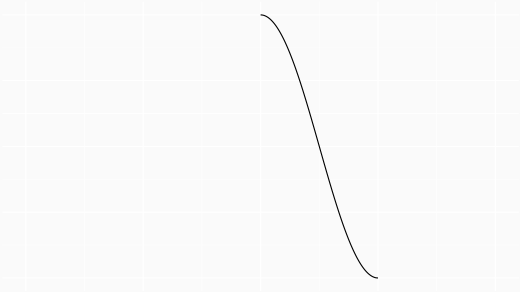
We think of our function on $[0, 1]$ as even 2-periodic functions for convenience. To do this, we reflect them across the y-axis and continue them periodically.



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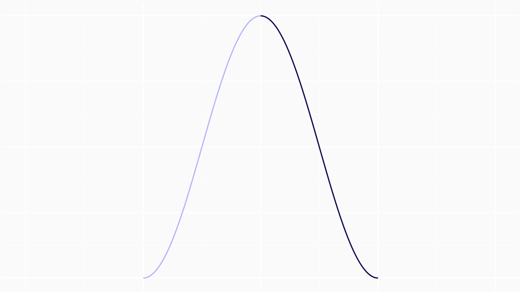

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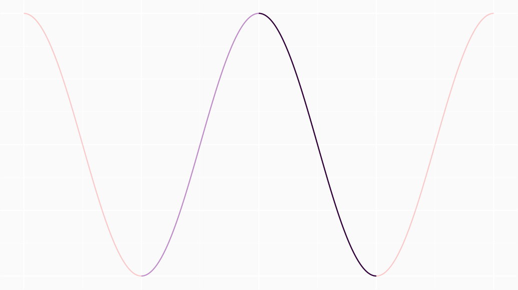

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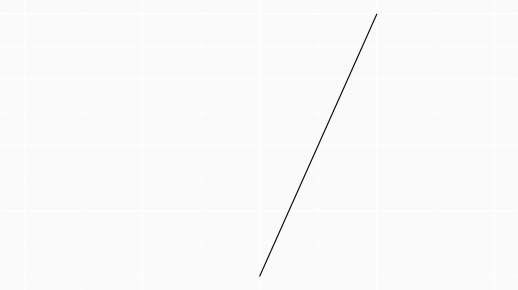

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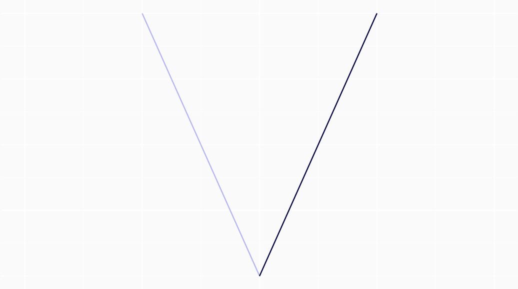

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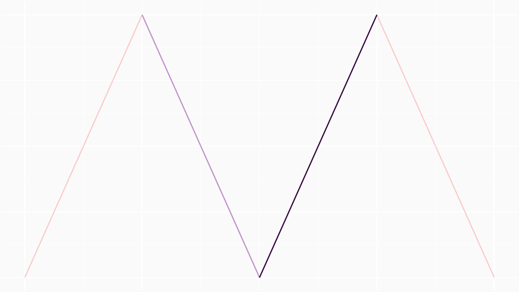

Self-adjoint operators are like *symmetric matrices*, but more general.
Like a symmetric matrices, their eigenvectors are an orthogonal basis for the space.

In this case, we're talking about the space of even 2-periodic functions.
So these eigenvectors are the even 2-periodic functions that solve this equation.

$$-\frac{d^2}{dx^2}\phi = \lambda\phi \quad \text{for some corresponding } \textit{eigenvalue} \quad \lambda \in \mathbb{R}$$

What are they?

Eigenvalues and Eigenvectors

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What are they?

$$\phi_j(x) = \sqrt{2}\cos(\pi j x) \quad \text{and} \quad \lambda_j = (\pi j)^2 \quad \text{for} \quad j = 0, 1, 2, \ldots$$

We know they're orthogonal. Not because we remember our trigonometry formulas from high school, but because eigenvectors of self-adjoint operators always are.

$$\langle \phi_j,\ \phi_k \rangle_{L_2} = 0 \ \text{ for } \ j \neq k$$

And we've scaled them so they're unit-length because it's convenient.

$$\langle \phi_j,\ \phi_j \rangle_{L_2} = 1$$

Our Fourier Series Characterization

Because our eigenvectors are a basis, we can write any function in our space as a combination of them.

$$m(x) = \sum_{j=0}^{\infty} m_j \phi_j(x)$$

Note that the *function* $m(x)$ and the *sequence of coefficients* m_j are different things. But they both describe the same function. That's why we use the same letter m.

Our model can be described as the set of these functions with coefficients in an ellipse defined in terms of the eigenvalues λ_j. It's an easy calculation.

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$$\begin{aligned} m \in \mathcal{M}^1 \quad \iff \quad B^2 &\geq \left\langle -\frac{d^2}{dx^2} m,\ m \right\rangle_{L_2} \\ &= \left\langle -\frac{d^2}{dx^2} \sum_j m_j \phi_j, \sum_k m_k \phi_k \right\rangle_{L_2} \\ &= \left\langle \sum_j m_j \lambda_j \phi_j, \sum_k m_k \phi_k \right\rangle_{L_2} \\ &= \sum_j \sum_k \lambda_j m_j m_k \langle \phi_j, \phi_k \rangle_{L_2} = \sum_j \lambda_j m_j^2. \end{aligned}$$

We did all this stuff for the model $\mathcal{M}^1$ with one bounded derivative.
But we can characterize models $\mathcal{M}^p$ with more bounded derivatives
using powers of our negated second derivative operator.

$$\mathcal{M}^p = \left\{ m \;\; : \left\langle \left(-\frac{d^2}{dx^2} \right)^p m, \; m \right\rangle_{L_2} \leq B^2 \right\}$$

This power has the same eigenvectors and powers of the eigenvalues.
That gives us the series characterization we're after.

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Homework Review

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Gaussian Width and Sobolev Models

A Convenient Bound on Width

Recall what gaussian width is. It's the mean of something.

$$\mathrm{w}(\mathcal{V}) = \mathrm{E}\, Z \quad \text{for} \quad Z = \max_{v \in \mathcal{V}} \frac{1}{n} \sum_{i=1}^{n} g_i v_i$$

Means are always less than root-mean-squares.

$$\mathrm{w}(\mathcal{V}) \le \mathrm{w}_2(\mathcal{V}) := \sqrt{\mathrm{E}\, Z^2} = \sqrt{(\mathrm{E}\, Z)^2 + \mathrm{Var}(Z)}$$

That root-mean-square $\mathrm{w}_2(\mathcal{V})$ is what we'll bound.

We'll bound the width of ...

1. The whole model
2. A neighborhood of zero
3. A neighborhood of an arbitrary point in the model.

Each is a small step from the last.

We'll assume X_i is uniformly distributed on $[0,1]$, i.e.,

$$\langle \phi_i, \phi_j \rangle_{L_2(P)} = \langle \phi_i, \phi_j \rangle_{L_2} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

When it's not, we can still get a similar bound. See the homework solution.

The Whole Model's Width

$$\mathrm{w}_2(\mathcal{M}) = \sqrt{\mathrm{E}\, Z^2} \quad \text{for} \quad Z = \max_{\substack{\text{sequences } m \\ \sum_j \lambda_j m_j^2 \le B^2}} \frac{1}{n} \sum_{i=1}^{n} g_i \left\{ \sum_j m_j \phi_j(X_i) \right\}.$$

Step 1. For all sequences m like this, via the Cauchy-Schwarz inequality,

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$$\begin{aligned}
\left| \frac{1}{n}\sum_{i=1}^n g_i \left\{ \sum_j m_j \phi_j(X_i) \right\} \right| &= \left| \sum_j m_j \left\{ \frac{1}{n}\sum_{i=1}^n g_i \phi_j(X_i) \right\} \right| \\
&= \left| \sum_j m_j \lambda_j^{1/2} \ \cdot \ \lambda_j^{-1/2} \left\{ \frac{1}{n}\sum_{i=1}^n g_i \phi_j(X_i) \right\} \right| \\
&\le \sqrt{\sum_j \left\{ m_j \lambda_j^{1/2} \right\}^2} \ \cdot \ \sqrt{\sum_j \left[\lambda_j^{-1/2} \left\{ \frac{1}{n}\sum_{i=1}^n g_i \phi_j(X_i) \right\} \right]^2} \\
&\le B \cdot \sqrt{\sum_j \lambda_j^{-1} \left\{ \frac{1}{n}\sum_{i=1}^n g_i \phi_j(X_i) \right\}^2}
\end{aligned}$$

The Whole Model's Width

$$\mathrm{w}_2(\mathcal{M}) = \sqrt{\mathrm{E}\, Z^2} \quad \text{where} \quad |Z| \le B \cdot \sqrt{\sum_j \lambda_j^{-1} \left\{ \frac{1}{n} \sum_{i=1}^{n} g_i \phi_j(X_i) \right\}^2}$$

Step 2. We can calculate the mean square of this bound on $|Z|$.

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$$\begin{aligned}
\mathrm{E}\, Z^2 &\le B^2 \sum_j \lambda_j^{-1}\, \mathrm{E} \left\{ \frac{1}{n} \sum_{i=1}^n g_i \phi_j(X_i) \right\} \left\{ \frac{1}{n} \sum_{i'=1}^n g_{i'} \phi_j(X_{i'}) \right\} \\
&= \frac{B^2}{n^2} \sum_j \lambda_j^{-1} \sum_{i=1}^n \sum_{i'=1}^n \mathrm{E}\, g_i g_{i'} \phi_j(X_i) \phi_j(X_j) \\
&\overset{(a)}{=} \frac{B^2}{n^2} \sum_j \lambda_j^{-1} \sum_{i=1}^n \sum_{i'=1}^n \mathrm{E}\, g_i g_{i'}\, \mathrm{E}\, \phi_j(X_i) \phi_j(X_j) \\
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&\overset{(c)}{=} \frac{B^2}{n^2} \sum_j \lambda_j^{-1} \sum_{i=1}^n 1 = \frac{B^2}{n} \sum_j \lambda_j^{-1}
\end{aligned}$$

(a) g and X are independent; (b) g_i and $g_{i'}$ are independent w/ mean zero; (c) $\mathrm{E}\, g_i^2 = \mathrm{Var}(g_i) = 1$ and $\mathrm{E}\, \phi_j(X_i)^2 = 1$.

The Whole Model's Width

$$\mathrm{w}_2(\mathcal{M}) \leq \sqrt{\frac{B^2}{n} \sum_j \lambda_j^{-1}} \quad \text{is our bound.}$$

There's a trick to this. Curves in our model are in one ellipse.

$$B^2 \geq \sum_j \lambda_j m_j^2$$

The constraint that we're near zero restricts our coefficients to another ellipse.

$$s^2 \geq \left\| \sum_j m_j \phi_j \right\|_{L_2}^2 = \left\langle \sum_j m_j \phi_j, \sum_k m_k \phi_k \right\rangle_{L_2} = \sum_{j,k} m_j m_k \langle \phi_j, \phi_k \rangle_{L_2} = \sum_j m_j^2.$$

In a neighborhood of zero within our model, *both constraints* are satisfied.
And so are linear combinations of them.

$$\sum_j m_j \phi_j \in \mathcal{M}_s \implies \frac{1}{B^2} \sum_j \lambda_j m_j^2 + \frac{1}{s^2} \sum_j m_j^2 \leq 1 + 1 = 2.$$

That tells that curves in our neighborhood are contained in another ellipse.

$$\mathcal{M}_s \subseteq \tilde{\mathcal{M}}_s := \left\{ \sum_j m_j \phi_j \;\; : \;\; \sum_j \tilde{\lambda}_j m_j^2 \leq 2 \right\} \quad \text{for} \quad \tilde{\lambda}_j = \frac{\lambda_j}{B^2} + \frac{1}{s^2}$$

And we can use our 'whole model' bound on this ellipse.

$$\mathrm{w}_2(\mathcal{M}_s) \leq \mathrm{w}_2(\tilde{\mathcal{M}}_s) \leq \sqrt{\frac{2}{n} \sum_j \left(\frac{\lambda_j}{B^2} + \frac{1}{s^2} \right)^{-1}}.$$

A Neighborhood of an Arbitrary Curve

There's a trick to this too. Think of our model as a ball in the *Sobolev seminorm*.

$$\mathcal{M} = \{m : \rho(m) \leq B\} \quad \text{where} \quad \rho\left(\sum_j m_j\phi_j\right) = \sqrt{\sum_j \lambda_j m_j^2}$$

Now let's think about our centered neighborhood.

$$\mathcal{M}_s - \mu^\star = \left\{m - \mu^\star \;\;:\;\; \rho(m) \leq B \text{ and } \|m - \mu^\star\|_{L_2} \leq s\right\}$$

This is contained in a neighborhood of zero by the triangle inequality.

$$\rho(m - \mu^\star) \leq \rho(m) + \rho(\mu^\star) \leq B + B$$

so

$$\mathcal{M}_s - \mu^\star \subseteq \left\{m - \mu^\star \;:\; \rho(m - \mu^\star) \leq 2B \quad \text{and} \quad \|m - \mu^\star\|_{L_2} \leq s\right\}.$$

This means we can use our last bound if we *double* B. Easy enough.

$$\mathrm{w}_2(\mathcal{M}_s) \leq \mathrm{w}_2(\tilde{\mathcal{M}}_s) \leq \sqrt{\frac{2}{n}\sum_j \left(\frac{\lambda_j}{(2B)^2} + \frac{1}{s^2}\right)^{-1}}.$$

Getting Concrete

Let's calculate this for our Sobolev model $\mathcal{M}^p$ by plugging in our eigenvalues.

$$\mathrm{w}_2(\mathcal{M}^p_s) \le \sqrt{\frac{2}{n}\sum_j \left(\frac{\lambda_j}{4B^2} + \frac{1}{s^2}\right)^{-1}} \quad \text{for} \quad \lambda_j = (\pi j)^{2p}$$

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Bounds and Approximations

1. Sum exceeds max.

$$\left(\frac{\lambda_j}{4B^2} + \frac{1}{s^2}\right)^{-1} \le \left\{\max\left(\frac{\lambda_j}{4B^2}, \frac{1}{s^2}\right)\right\}^{-1} = \min\left(\frac{4B^2}{\lambda_j},\ s^2\right)$$

2. Integral approximation.

$$\sum_j \min\left(\frac{4B^2}{\lambda_j},\ s^2\right) \approx \int_0^\infty \min\left(\frac{4B^2}{\lambda_x}, s^2\right) dx$$

Conclusion

$$\mathrm{w}_2(\mathcal{M}_s^p) \lesssim \sqrt{\frac{2}{n}\int_0^\infty \min\{4B^2(\pi x)^{-2p},\ s^2\}\, dx}$$

$$\le \sqrt{\frac{8B^2}{n}\int_0^\infty \min\{(\pi x)^{-2p},\ s^2\}\, dx} \quad \text{for} \quad B \ge 1/2$$

What is this really?

$$\mathrm{w}_2(\mathcal{M}_s^p) \leq \sqrt{\frac{8B^2}{n} \int_0^\infty \min\{(\pi x)^{-2p},\ s^2\} dx} \quad \text{for} \quad B \geq 1/2$$

The integral has two parts.

1. The beginning, where $(\pi x)^{-2p}$ is big and we're just integrating s^2.
2. The end, where $(\pi x)^{-2p}$ is small and we're integrating that.

When does the end start?

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It starts when $x > \pi^{-1}s^{-1/p}$. Let's do it.

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$$\begin{aligned}
&= \int_0^{\pi^{-1}s^{-1/p}} s^2 \quad + \quad \int_{\pi^{-1}s^{-1/p}}^\infty \pi^{-2p}x^{-2p}dx \\
&= \pi^{-1}s^{2-1/p} \quad + \quad \pi^{-2p}\left.\frac{x^{1-2p}}{1-2p}\right|_{\pi^{-1}s^{-1/p}}^\infty && \text{if } p > 1/2\text{, otherwise } \infty \\
&= \pi^{-1}s^{2-1/p} \quad + \quad \pi^{-2p}\frac{\pi^{2p-1}s^{2-1/p}}{2p-1} = c_p s^{2-1/p} && \text{for} \quad c_p = \pi^{-1}\{1 + 1/(2p-1)\}.
\end{aligned}$$

Our width bound is proportional to $1/\sqrt{n}$ times the integral's square root.

$$\mathrm{w}(\mathcal{M}_s^p) \lesssim Bn^{-1/2}s^{1-1/2p}.$$

An Error Bound

To bound our least squares estimator's error, we do what we always do.
We find the smallest solution we can to this inequality.

$\|\hat{\mu} - \mu^{\star}\| \leq s$ w.p $1 - \delta$ if $s^2 \geq 2\sigma c_\delta \, \mathrm{w}(\mathcal{M}_s^p)$ and therefore if $s^2 \geq c_\delta' B n^{-1/2} s^{1-1/2p}$

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And this means that we gain a decimal point of precision with ...

- $10^3 = 1000$ times more data using a model with $p=1$ bounded derivative.
- $10^{2.50} \approx 300$ times more data using a model with $p=2$ bounded derivatives.
- $10^{2.33} \approx 200$ times more data using a model with $p=3$ bounded derivatives.
- $10^{2.25} \approx 175$ times more data using a model with $p=4$ bounded derivatives.

This is starting to look more possible. But getting into models we don't understand.
What do 3 or 4 bounded derivatives look like? This'll be a problem soon.

Multidimensional Sobolev Models

The Isotropic Sobolev Model

To get a multidimensional generalization of our ($p = 1$) Sobolev model, we can replace the squared derivative with the *squared norm* of the gradient.

$$\mathcal{M}^1 = \{m : \rho_{\text{-}\Delta}(m) \le B\} \quad \text{where} \quad \rho_{\text{-}\Delta}(m) = \sqrt{\int_{[0,1]^d} \|\nabla m(x)\|^2 \, dx}.$$

Much like in the univariate case, we can use integration by parts to get an equivalent definition in terms of a self-adjoint operator.

$$\mathcal{M}^1 = \{m : \rho_{\text{-}\Delta}(m) \le B\} \quad \text{where} \quad \rho_{\text{-}\Delta}(m) = \sqrt{\langle \text{-}\Delta^p \, m, m \rangle_{L_2}}.$$

That operator is the second derivative's simplest higher-dimensional generalization.

The Laplacian $$\text{-}\Delta \, m = -\frac{\partial^2}{\partial x_1^2} m(x) - \ldots - \frac{\partial^2}{\partial x_d^2} m(x)$$

It's a self-adjoint operator on functions that are even and 2-periodic along each axis.

$$f(\pm x_1, \ldots, \pm x_d) = f(x_1 + 2j_1, \ldots, x_j + 2j_d) = f(x_1, \ldots, x_d) \quad \text{for} \quad \underbrace{j \in \mathbb{Z}^d}_{\text{integer vectors}}.$$

Because this operator self-adjoint, we know it has an orthogonal basis of eigenvectors.

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Anybody want to guess?

Eigenvectors and Eigenvalues

Because this operator self-adjoint, we know it has an orthogonal basis of eigenvectors.

The Laplacian $$-\Delta\, m = -\frac{\partial^2}{\partial x_1^2} m(x) - \ldots - \frac{\partial^2}{\partial x_d^2} m(x)$$

Anybody want to guess?

They're *products* of cosines.

$\phi_j(x) = \cos(\pi j_1 x_1) \cdots \cos(\pi j_d x_d)$ with eigenvalue $\lambda_j = (\pi \|j\|_2)^2$ for $\underbrace{j \in \mathbb{Z}^d}_{\text{integer vectors}}$.

There are versions for higher order derivatives.

$$\mathcal{M}^p = \{m : \rho_{\text{-}\Delta^p}(m) \le B\} \quad \text{where} \quad \rho_{\text{-}\Delta^p}(m) = \sqrt{\langle \text{-}\Delta^p\, m, m\rangle_{L_2}}$$

And Fourier series representations.

$$\mathcal{M}^p = \left\{ \sum_{j \in \mathbb{Z}^d} m_j \phi_j \ : \sum_{j \in \mathbb{Z}^d} \lambda_j^p \ m_j^2 \le B^2 \right\} \quad \text{for} \quad \phi_j(x) = \cos(\pi j_1 x_1) \cdots \cos(\pi j_d x_d)$$

$$\text{and} \quad \lambda_j = (\pi \|j\|_2)^2.$$

You can derive all this stuff the same way as the univariate case.

The Gaussian Width of a Neighborhood

Abstractly, width is the same thing. All we used before were the eigenvalues.

$$\mathrm{w}(\mathcal{M}_s^p) \le \sqrt{\frac{8B^2}{n}\sum_j \min\left\{\lambda_j^{-1},\ s^2\right\}} \quad \text{for} \quad \lambda_j = (\pi\|j\|_2)^{2p}.$$

- But now we're summing more or them, spreading out in all d directions.
- This means we see the same value of λ_j^{-1} in the sum multiple times.
- Same $\|j\|_2$, different j.

Integral approximation makes it easy to 'count' these copies.

$$\mathrm{w}(\mathcal{M}_s^p) \lesssim \sqrt{\frac{8B^2}{n}\int_{x\in\mathbb{R}^d} \min\{(\pi\|x\|_2)^{-2p},\ s^2\}dx}$$

- The 'number of copies' gets larger as $\|x\|_2$ does.
- To be precise, it's the surface area of the sphere of radius $r = \|x\|_2$
- And if we change variables to polar coordinates, the integral is easy.

Step 1. Reduce it to a one-dimensional integral.

$$\mathrm{w}(\mathcal{M}_s^p)^2 \lesssim \frac{8B^2}{n} \int_{x \in \mathbb{R}^d} \min\left\{(\pi \|x\|_2)^{-2p}, s^2\right\} dx$$

in rectangular coordinates

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$$= \frac{8B^2}{n} \int \left[\int r^{d-1} \min\left\{(\pi r)^{-2p}, s^2\right\} dr \right] d\theta_1 \ldots \theta_{d-1} \qquad \text{in polar coordinates}$$

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$$= \frac{8B^2}{n} \left[\int r^{d-1} \min\{(\pi r)^{-2p}, s^2\} \, dr \right] \underbrace{\int 1 \, d\theta_1 \dots \theta_{d-1}}_{\substack{\text{sphere surface area} \\ 2\pi^{d/2} / \, \Gamma(d/2) \leq 35}}$$ $\left[\int \dots \right]$ is constant in θ

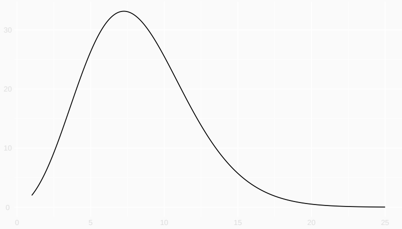

Figure 2: sphere surface area vs. dimension

The Integral

Step 2. Calculate the one-dimensional integral. This should be familiar.

$$\mathrm{w}(\mathcal{M}_s^p)^2 \lesssim \frac{8B^2}{n} \cdot \frac{2\pi^{d/2}}{\Gamma(d/2)} \cdot \int r^{d-1} \min\{(\pi r)^{-2p}, s^2\}\, dr$$

The integral has two parts.

1. The beginning, where $(\pi r)^{-2p}$ is big and we're just integrating $r^{d-1} \times s^2$.
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When does the end start?

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It starts when $r > \pi^{-1} s^{-1/p}$. Let's do it.

$$= \int_0^{\pi^{-1}s^{-1/p}} r^{d-1} s^2\, dr \quad + \quad \int_{\pi^{-1}s^{-1/p}}^{\infty} \pi^{-2p} r^{d-1-2p}\, dr$$

$$= s^2 \frac{r^d}{d}\Big|_0^{\pi^{-1}s^{-1/p}} \quad + \quad \pi^{-2p} \frac{r^{d-2p}}{d-2p}\Big|_{\pi^{-1}s^{-1/p}}^{\infty}$$

if $p > d/2$, otherwise ∞

$$= \frac{\pi^{-d} s^{2-d/p}}{d} \quad + \quad \frac{\pi^{-d} s^{2-d/p}}{2p-d} = c_{d,p} s^{2-d/p}$$

for $c_{d,p} = \frac{\pi^{-d}}{d}\left\{1 + \frac{1}{\frac{2p}{d} - 1}\right\}$

Summary.
Our width bound is proportional to $n^{-1/2}\ s^{1-d/2p}$.

$$\mathrm{w}(\mathcal{M}_s^p)^2 \lesssim \frac{8B^2}{n} \cdot \frac{2\pi^{d/2}}{\Gamma(d/2)} \cdot c_{d,p} s^{2-d/p}$$

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We've essentially solved this in the 1D case.
But now **smoothness is relative to dimension**: p/d is the new p.

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Derivation.

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- $10^4 = 10,000$ times more data using a model with $p = d/2$ bounded derivatives.
- $10^3 = 1000$ times more data using a model with $p = d$ bounded derivatives.
- $10^{2.50} \approx 300$ times more data using a model with $p = 2d$ bounded derivatives.
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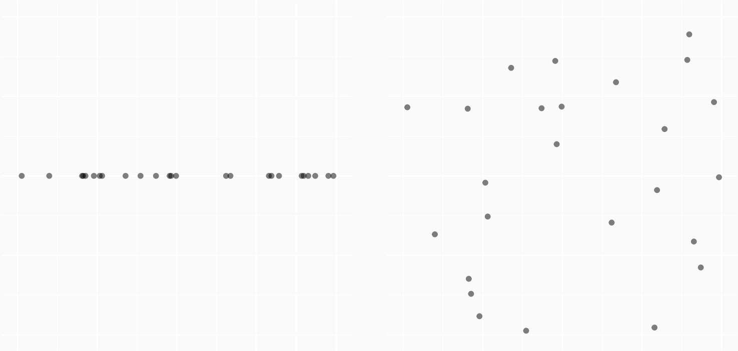
- $10^{2.25} \approx 175$ times more data using a model with $p = 4d$ bounded derivatives.

Smoothness doesn't count for much if it's spread over many dimensions.
Even if we've got *tons* of data, we need $3+$ derivatives in $3+$ dimensions.
That's the **curse of dimensionality**.

Intuition

If two points are close, a smooth functions's values at them will be close.
But this isn't very useful if our observations are far apart.
And higher-dimensional observations *do* tend to be further apart.



Left Uniformly distributed points in the unit interval.
Right Uniformly distributed points in the square interval.

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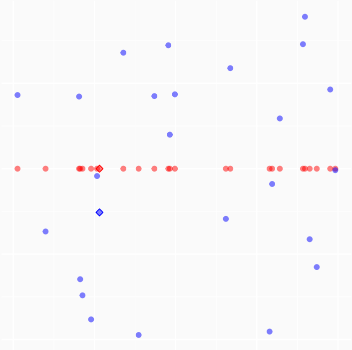

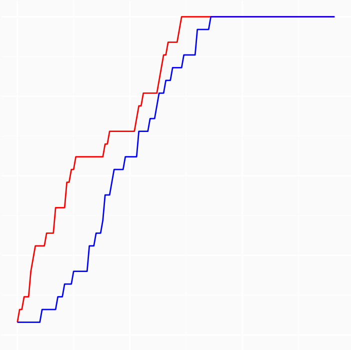

Left. As before, but overlaid.
Right. Fraction of points (y) within a distance (x) of one of them ($\diamond$).

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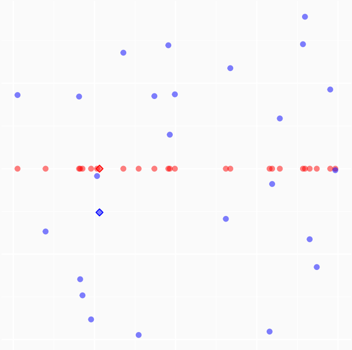

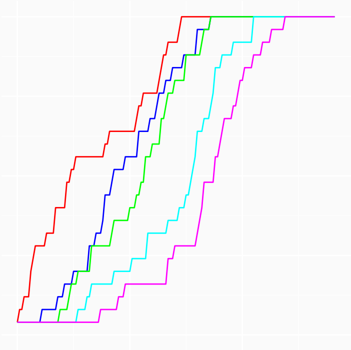

Left. As before, but overlaid.
Right. Fraction of points (y) within a distance (x) of one of them ($\diamond$).
Extra curves are for the unit 3/4/5-dimensional cubes.

This looks bad

$$n^{-1/(2+d/p)} \quad \text{is our rate of convergence.}$$

The cube-root interpretation.

- With one-dimensional data, we've been getting $n^{-1/3}$ rates.
  - That's more 1 digit of precision / $1000\times$ more observations.
  - It's going from a study that enrolls the students in one intro class to everyone at Emory, UGA and Tech.
  - That's a lot, but maybe it's what we're used to and we can accept that.
  - It's what we got for monotone, bounded variation, and lipschitz regression.
- With two-dimensional data, we can do that by constraining *second derivatives*.
- With data in $3+$ dimensions, we'd need to constrain 3rd derivatives. That's bad.
  - We don't have much intution for 3rd derivatives
  - So we'd be relying on assumptions we essentially don't understand.
- People say the curse is a *high dimensional* phenomenon. It's not.
- By this standard, 3 dimensional data — most data — is high dimensional.

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The fourth-root interpretation.

- If we want to estimate something like an average treatment effect— a number rather than a curve—things aren't quite as bad.
- Clever estimators like the *R-Learner* amplify our precision.
- They make it possible to get a $n^{-1/2}$ rate estimates the effect.
    - That's more 1 digit of precision / $100\times$ more observations.
    - It's going from a study that enrolls the students in one intro class to everyone at Emory. Not terrible.
    - And there's no way to do better, even with extremely strong assumptions.
    - That's the rate at which sample averages converge.
- What we need to do that is $n^{-1/4}$ rate estimates of a few curves. π and β.
- We can do that with constrained pth derivatives for $p = d/2$.
- i.e. we can do without third derivatives until we've got $5+$-dimensional data.

This looks bad

$n^{-1/(2+d/p)}$ is our rate of convergence.

The everyone in the world interpretation

- Suppose we've run a study on a 80-student intro class.
- And we're now going to rerun it on everyone in the world.
- About 8 billion people. A hundred million (10^8) times more.
- That's a hard thing to do, so we want a big return. Two more digits.
- We can do that if we're estimating curve in K-or-fewer dimensions. What's K?

Good news?

The Isotropic Sobolev model may be the wrong model to use.
It's popular, but it's a terrible model for most things.

$$\mathcal{M} = \left\{ m : \frac{1}{2^d} \int_{[-1,1]^d} \|\nabla m(x)\|_2^2 \le B^2 \right\}$$

The problem is that it's isotropic, i.e. rotation invariant. Almost.

You can show it using the chain rule. If $m_R(x) = m(Rx)$ for a rotation matrix R,

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$$\begin{aligned} \nabla m_R(x) = R\,\nabla m(Rx) \implies \|\nabla m_R(x)\|_2^2 &= \langle R\,\nabla m(Rx),\ R\,\nabla m(Rx)\rangle_2 \\ &= \langle \underbrace{R^T R}_{=I}\,\nabla m(Rx),\ \nabla m(Rx)\rangle_2 = \|\nabla m(Rx)\|_2^2 \end{aligned}$$

And our squared Sobolev norm is this integrated over the unit cube.
That's $\|\nabla m\|_2^2$ integrated over a rotation of that cube.

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Intuition.

We pay the same for variation along every unit-length combination of covariates.

$$\begin{pmatrix} \text{income74} \\ \text{income75} \end{pmatrix} \quad \text{rotates to} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} \text{income74} - \text{income75} \\ \text{income74} + \text{income75} \end{pmatrix}.$$

We usually expect different amounts of variation along different combinations.
The curse hits, in part, because the model doesn't encode our assumptions.

An Overcorrection

Additive models *only* allow variation along the axes.

$$\mathcal{M} = \left\{ m(x) = m_1(x_1) + \ldots + m_d(x_d) \quad : \quad \|m_1'\|_{L_2}^2 + \ldots \|m_d'\|_{L_2}^2 \leq B^2 \right\}$$

We take the contributions of each covariate and sum them up.

- What's nice is that they don't suffer from the curse of dimensionality.
- We always get error bounds comparable to what we'd get in $1D$.
- What isn't is that they can't fit all that much.

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- You might think average income in 74 and 75 predicts income in 76. Additive.
- Maybe you'll earn a bit more if you were on an upward trajectory. Maybe Additive.
- Maybe you'll also earn much more if you took a big dip in 75.
  e.g. you spent part of 75 unemployed. That's not additive.

Middle Ground

Sobolev Models with Higher Order *Mixed Partials* are somewhere between these. They penalize off-axis variation *more*, but still allow it.

This is a 2D version. We include the mixed partial.

$$\mathcal{M} = \left\{ m \ : \ \frac{1}{4} \int_{[-1,1]^2} \|\nabla m(x)\|^2 + \left\{ \frac{\partial^2}{\partial x_1 \partial x_2} m(x) \right\}^2 \leq B^2 \right\}$$

And this is the general case. We include *all* mixed partials.

$$\mathcal{M} = \left\{ m \ : \ \frac{1}{2^d} \int_{[-1,1]^d} \sum_{\substack{k \in \mathbb{Z}_+^d \\ \max_{i \leq d} k_i = 1}} \left\{ \frac{\partial^{\sum_i k_i}}{\partial x_1^{k_1} \dots \partial x_d^{k_d}} m(x) \right\}^2 \leq B^2 \right\}$$

A Picture

Exercise

Bound the width of a neighborhood in this model.

$$\mathcal{M} = \left\{ m(x) = m_1(x_1) + \ldots + m_d(x_d) \quad : \quad \|m_1'\|_{L_2}^2 + \ldots \|m_d'\|_{L_2}^2 \le B^2 \right\}$$

Exercise

Bound the width of a neighborhood in this model.

$$\mathcal{M} = \left\{ m \ : \ \frac{1}{4}\int_{[-1,1]^2} \|\nabla m(x)\|^2 + \left\{ \frac{\partial^2}{\partial x_1 \partial x_2} m(x) \right\}^2 \le B^2 \right\}$$