Machine Learning Theory

Multivariate Sobolev Regression

David A. Hirshberg

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Emory University

TODO

- Illustrate Slower Rate of Convergence for 2D Data (image) Empirically [Zero image; Gaussian Bump]
- Do Additive Model Example (Maybe prove truncation result?) also with Rate of Convergence
- Introduce Mixed Partials Model in Lab [Do Calculations Yourself; Main lab content = finding/playing with images]

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

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.

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

Eigenvectors and Eigenvalues

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

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Anybody want to guess?

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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 $j \in \mathbb{Z}^d$.

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.

The Integral

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

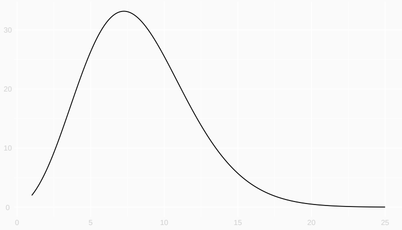

Figure 1: sphere surface area vs. dimension

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 $r^{d-1} \times s^2$.
2. The end, where $(\pi r)^{-2p}$ is small and we're integrating $r^{d-1}\times$ that.

When does the end start?

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

$$= s^2 \frac{r^d}{d}\Big|_0^{\pi^{-1}s^{-1/p}} \quad + \quad \pi^{-2p} \frac{r^{d-2p}}{d-2p}\Big|_{\pi^{-1}s^{-1/p}}^{\infty} \qquad \text{if } p > d/2\text{, otherwise } \infty$$

$$= \frac{\pi^{-d}s^{2-d/p}}{d} \quad + \quad \frac{\pi^{-d}s^{2-d/p}}{2p-d} = c_{d,p}s^{2-d/p} \qquad \text{for } c_{d,p} = \frac{\pi^{-d}}{d}\left\{1 + \frac{1}{\frac{2p}{d} - 1}\right\}$$

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

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

An Error Bound

To bound our least squares estimator's error, we do what we always do.

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

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

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

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Derivation.

$$\begin{aligned} s^2 &\gtrsim n^{-1/2} s^{1-d/2p} && \text{or equivalently} \\ s^{1+d/2p} &\gtrsim n^{-1/2} && \text{or equivalently} \\ s &\gtrsim n^{-1/\{2(1+d/2p)\}} = n^{-1/(2+d/p)}. \end{aligned}$$

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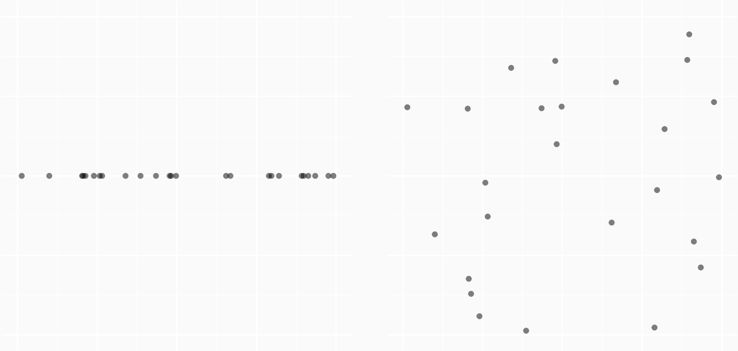
- $10^4 = 10,000$ times more data using a model with $p = d/2$ bounded derivatives.
- $10^3 = 1000$ times more data using a model with $p = d$ bounded derivatives.
- $10^{2.50} \approx 300$ times more data using a model with $p = 2d$ bounded derivatives.
- $10^{2.33} \approx 200$ times more data using a model with $p = 3d$ bounded derivatives.
- $10^{2.25} \approx 175$ 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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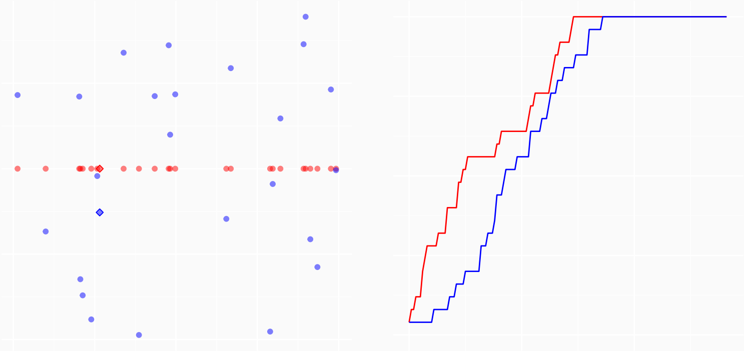

Left. As before, but overlaid.
Right. Fraction of points (y) within a distance (x) of one of them ($\diamond$).

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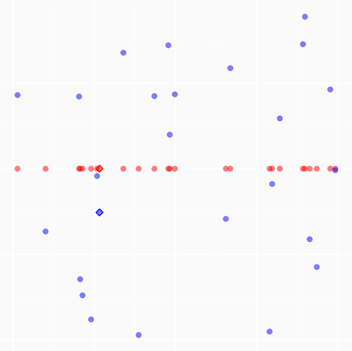

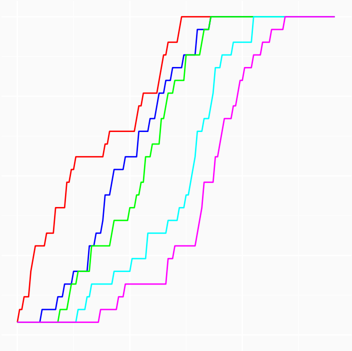

Left. As before, but overlaid.
Right. Fraction of points (y) within a distance (x) of one of them ($\diamond$).
Extra curves are for the unit 3/4/5-dimensional cubes.

This looks bad

$n^{-1/(2+d/p)}$ 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.

This looks bad

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

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.

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

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.

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.

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

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

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

A Picture

Exercise

Bound the width of a neighborhood in this model.

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Bound the width of a neighborhood in this model.

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