Machine Learning Theory

Sobolev Regression

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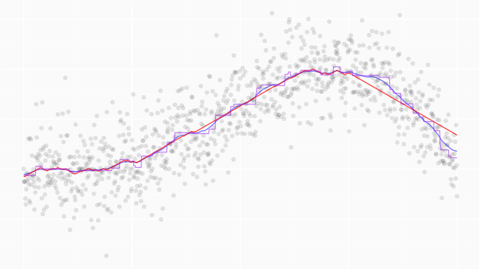
Smoothness constraints



So far, we've talked about two models based on smoothness constraints.

$$\mathcal{M}_1 = \{m \;:\; \|m'\|_{L_1} \le B\} \qquad \text{The Bounded Variation Model}$$

$$\mathcal{M}_\infty = \{m \;:\; \|m'\|_{L_\infty} \le B\} \qquad \text{The Lipschitz Model}$$

Today we'll look at one that's similar, but more convenient: the *Sobolev* model.

$$\mathcal{M}_2 = \{m \;:\; \|m'\|_{L_2} \le B\}.$$

It bounds the mean square of the derivative's absolute value, not the max or mean.
It's 'between' the other two. I'll leave the proof of this as an exercise.

We'll focus on the $B = 1$ case today to keep the math simple.

Exercise

$$\mathcal{M}_\infty \subseteq \mathcal{M}_2 \subseteq \mathcal{M}_1$$

Prove it! Use the 'for differentiable functions' definitions of these models.

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$$\mathcal{M}_\infty \subseteq \mathcal{M}_2 \subseteq \mathcal{M}_1$$

Prove it! Use the ‘for differentiable functions’ definitions of these models.

Hint. It’s equivalent to show the corresponding seminorms have the reverse order.

$$\rho_p(m) = \|m'\|_{L_p} \quad \text{satisfies} \quad \rho_1(m) \leq \rho_2(m) \leq \rho_\infty(m).$$

Fourier Series Representation

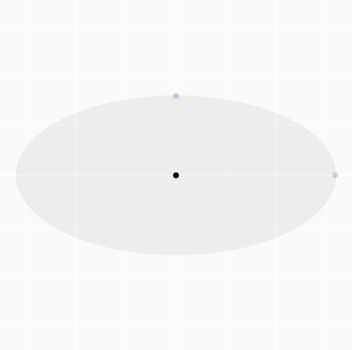
There's an equivalent definition in terms of an *orthogonal basis* for functions on $[0,1]$.

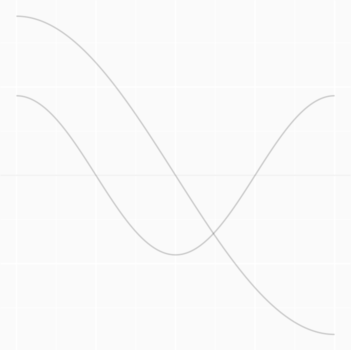
$$\mathcal{M} = \left\{ m : \int_0^1 m'(x)^2 \, dx \le 1 \right\} = \left\{ \sum_{j=0}^{\infty} m_j \phi_j(x) : \sum_{j=0}^{\infty} \lambda_j m_j^2 \le 1 \right\}$$

$$\text{where} \qquad \int_0^1 \phi_j(x)\phi_k(x)\, dx = 0 \quad \text{for} \quad j \ne k.$$

- We call this a *Fourier series representation*.
- It makes stuff looks a bit like what you'd see in intro classes.
- We can think of the *higher order terms* — ϕ_j where λ_j is large — much like we'd think about quadratic terms, interactions, etc., in linear regression.

In fact, these basis functions are *cosines* of increasing frequency.



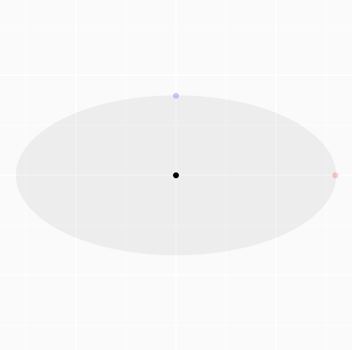


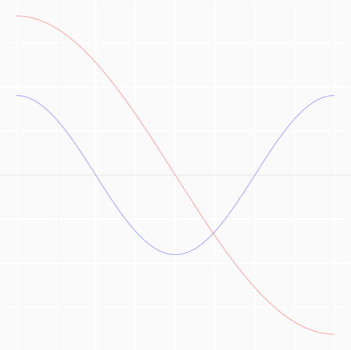
$$\mathcal{M} = \left\{ \sum_{j=0}^{\infty} m_j \phi_j(x) \ : \ \sum_{j=0}^{\infty} \lambda_j m_j^2 \leq 1 \right\}$$

for $\phi_j(x) = \sqrt{2}\cos(\pi j x)$ and $\lambda_j = \pi^2 j^2$.

Q. What's the correspondence between coefficients and curves?

Cosine Series





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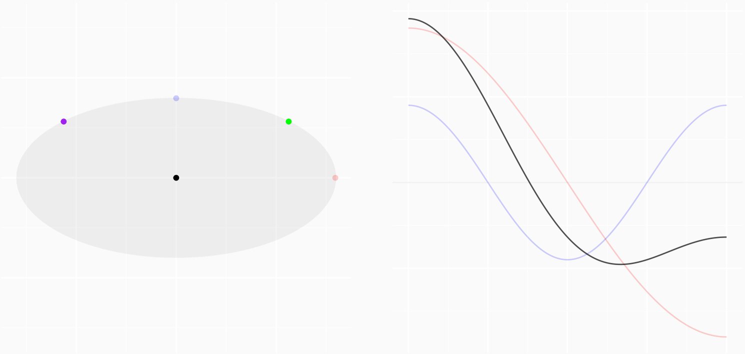

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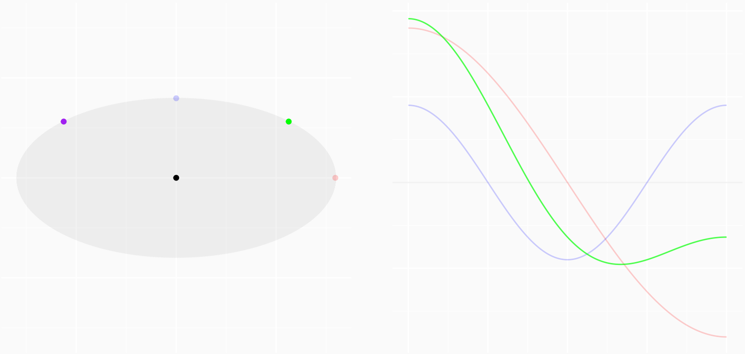
Q. Have I drawn the curve with the green coefficients or the purple ones?



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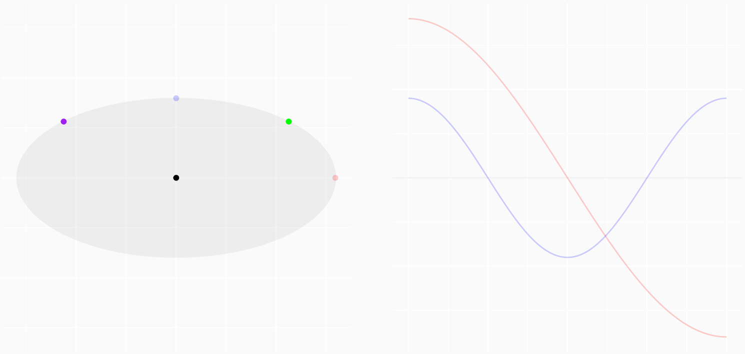

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Exercise. Draw the curve with the purple coefficients.

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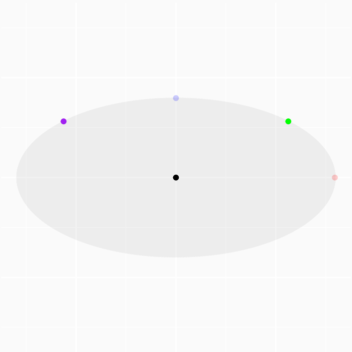

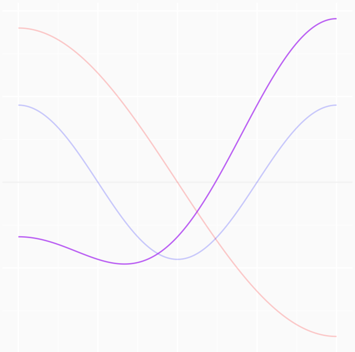

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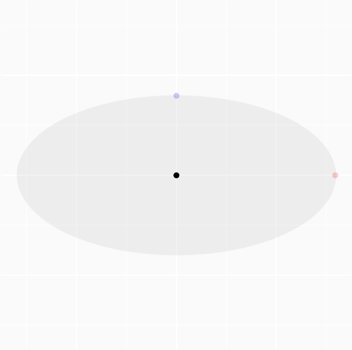

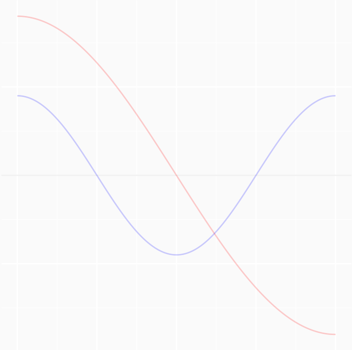

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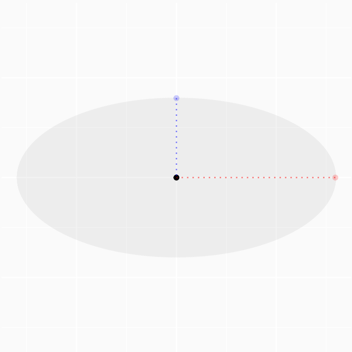

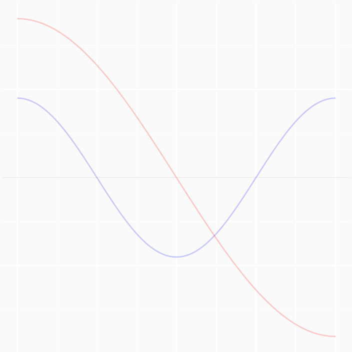

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Q. What's the geometric significance of $\frac{1}{\sqrt{\lambda_j}}$? **A.** They're ellipse radii.

Where the Series Representation Comes From

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.

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

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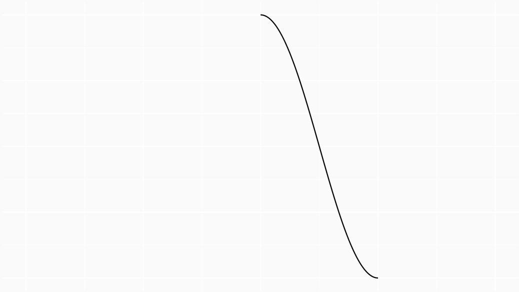
We think of our function on $[0, 1]$ as even 2-periodic functions for convenience.
To do this, we reflect them across the y-axis and continue them periodically.



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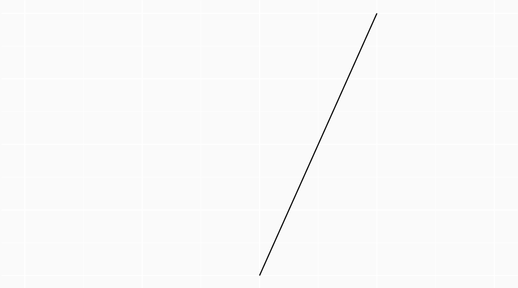

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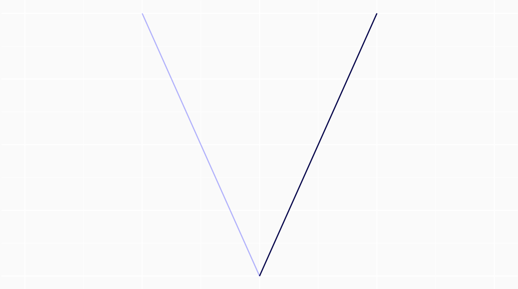

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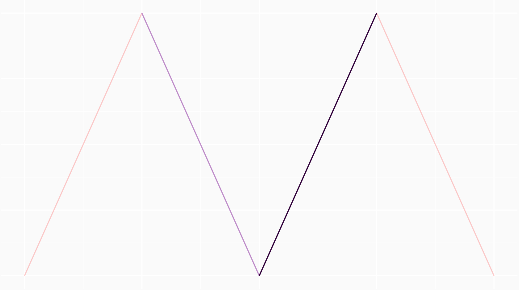
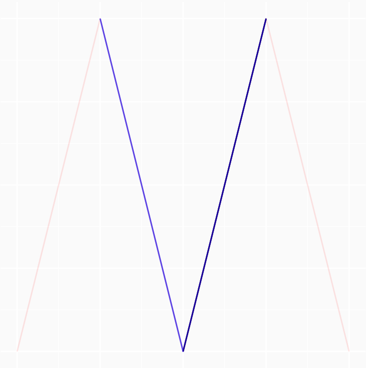


Claim. The *adjoint* of $\frac{d}{dx}$ is $-\frac{d}{dx}$ when we're using the inner product $\langle u, v\rangle_{L_2} = \int_0^1 u(x)v(x)\,dx$ on the space of even 2-periodic functions.

Starting Point. An equivalent way to write our inner product.

$$\begin{aligned}
\langle u, v\rangle_{L_2} &= \int_0^1 u(x)v(x)\,dx \\
&= \frac{1}{2}\int_{-1}^{0} u(x)v(x)\,dx + \frac{1}{2}\int_0^1 u(x)v(x)\,dx \\
&= \frac{1}{2}\int_{-1}^{1} u(x)v(x)\,dx
\end{aligned}$$



Review: The Integration by Parts Argument

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Proof.

$$\begin{aligned}
\left\langle u,\ \frac{d}{dx}v\right\rangle_{L_2} &= \frac{1}{2}\int_{-1}^{1} u(x)v'(x)\,dx \\
&= \frac{1}{2}u(x)v(x)\ |_{-1}^{1} - \frac{1}{2}\int_{-1}^{1} u'(x)v(x) && \text{integrating by parts} \\
&= 0 - \frac{1}{2}\int_{-1}^{1} u'(x)v(x) && \text{using periodicity} \\
&= \left\langle -\frac{d}{dx}u,\ v\right\rangle_{L_2}
\end{aligned}$$

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Implication. $-\frac{d^2}{dx^2}$ is self-adjoint.

$$-\frac{d^2}{dx^2} = T^\star T \qquad \text{for} \quad T = \frac{d}{dx}$$

$$\langle u, T^\star Tv\rangle_{L_2} = \langle Tu, Tv\rangle_{L_2} = \langle T^\star Tu, v\rangle \qquad \text{for any linear operator } T$$

Eigenvalues and Eigenvectors

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.

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

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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.

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

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What about sines?

- They're not in our space. $\sin(\pi j x)$ isn't even.
- We use a space of even functions because reflection gives us even functions.

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Why not other $j \in \mathbb{R}$?

- They're not in our space either. $\cos(\pi jx)$ is only 2-periodic for integer j.
- And periodic extension gives us periodic functions.

Our Fourier Series Characterization

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

$$m(x) = \sum_{j=0}^{\infty} m_j \phi_j(x) \quad \text{with} \quad \langle \phi_j, \phi_k \rangle_{L_2} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{otherwise} \end{cases}.$$

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.

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

Generalizations

Generalizations

More and Less Smooth Models

Smoother Models

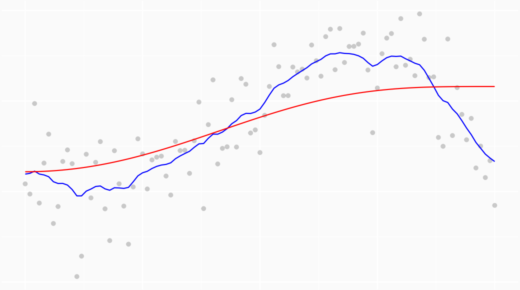

Figure 1: Least squares estimators for s=1 and s=2

- We did all this stuff for the model $\mathcal{M}^1$ with one bounded derivative.
- But we can characterize models $\mathcal{M}^k$ with more bounded derivatives easily.
- We use the same basis and powers of the same eigenvalues.

$$\mathcal{M}^k = \left\{ m \ : \|m^{(k)}(x)\|_{L_2} \le 1 \right\} = \left\{ m(x) = \sum_{j=0}^{\infty} m_j \phi_j(x) \ : \ \sum_{j=0}^{\infty} \lambda_j^k m_j^2 \le 1 \right\}$$

$$\mathcal{M}^k = \left\{ m : \|m^{(k)}(x)\|_{L_2}^2 \, dx \le 1 \right\} = \left\{ \sum_{j=0}^{\infty} m_j \phi_j(x) \ : \ \sum_{j=0}^{\infty} \lambda_j^k m_j^2 \le 1 \right\}.$$

Why?

The relevant seminorm involves the kth power of the second derivative operator.

$$\|m^{(k)}(x)\|_{L_2}^2 = \left\langle -\frac{d^2}{dx^2} \underset{k \text{ times}}{\ldots} - \frac{d^2}{dx^2} m, \ m \right\rangle \quad \text{via integration by parts}$$

And the kth power of any operator T has …

- the same eigenvectors ϕ_j as T itself.
- eigenvalues λ_j^k that are powers of the eigenvalues of T.

Fractional-Derivative Models

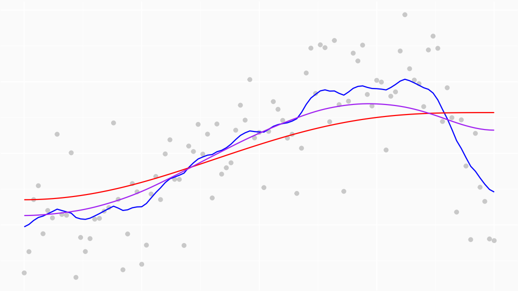

Figure 2: Least squares estimators for s=1, s=2, and s=3/2

$$\mathcal{M}^k = \left\{ m : \|m^{(k)}(x)\|_{L_2}^2 \, dx \le 1 \right\} = \left\{ \sum_{j=0}^{\infty} m_j \phi_j(x) \ : \ \sum_{j=0}^{\infty} \lambda_j^k m_j^2 \le 1 \right\}.$$

What happens if we take $k = 1/2$? Or $k = 3/2$? Or $k = 27/13$?

- There isn't really an obvious definition of $m^{(k)}$ for non-integer k.
- But we the Fourier-series definition of our model $\mathcal{M}^k$ still makes sense.

Generalizations

Multidimensional 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.

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?

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

integer vectors

Smoother Isotropic Sobolev Models

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.

Generalizations

The Gaussian Sobolev Model

What if we want to model functions on $\mathbb{R}$ instead of $[0,1]$?

We can define a similar model using a different inner product.
Like the $L_2(P)$ inner product where P is the standard normal distribution.

$$\begin{aligned}\langle u, v\rangle &= \mathrm{E}\, u(X)v(X) \quad \text{for} \quad X \sim N(0,1) \\ &= \int_{-\infty}^{+\infty} u(x)v(x)\phi(x)\,dx \quad \text{for} \quad \phi(x) = (1/\sqrt{2\pi})e^{-x^2/2}\end{aligned}$$

We get a space of functions m from $\mathbb{R} \to \mathbb{R}$ that don't grow too fast as x approaches $\pm\infty$.

$$\mathcal{M} = \left\{ m \;:\; \lim_{x \to \pm\infty} m(x)^2\phi(x) = 0 \text{ and } \rho(m) \leq 1 \right\}$$

$$\text{for} \quad \rho(m) = \sqrt{\int_{-\infty}^{+\infty} \left\{ \frac{d}{dx} m(x) \right\}^2 \phi(x)\; dx}$$

A Related Self-Adjoint Operator

Q. Is there a self-adjoint operator that characterizes this model?

$$\|m'\|^2 = \int_{-\infty}^{+\infty} m'(x)^2 \phi(x)\,dx \stackrel{?}{=} \langle Sm,\ m\rangle$$

A. Yes. It's $Su = xu' - u''$. Prove it!

Tip. Use the 'gaussian integration by parts formula' below to show that the adjoint of $T = \frac{d}{dx}$ satisfies $T^\star u = xu - u'$.

$$\begin{aligned}
\int_{-\infty}^{+\infty} u'(x)v(x)\phi(x)\,dx &= u(x)v(x)\phi(x)\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} u(x)\{v\phi\}'(x)\,dx \\
&= 0 - \int_{-\infty}^{+\infty} u(x)\{v\phi\}'(x)\,dx \\
&= 0 - \int_{-\infty}^{+\infty} u(x)\{v'\phi + v\phi'(x)\}\,dx \\
&= \int_{-\infty}^{+\infty} u(x)xv(x)\phi(x)\,dx - \int_{-\infty}^{+\infty} u(x)v'(x)\phi(x)\,dx \qquad \text{because } \phi'(x) =
\end{aligned}$$

$$
\begin{aligned}
\mathcal{M} &= \left\{ m \;:\; \lim_{x \to \pm\infty} m(x)^2 \phi(x) = 0 \;\text{ and }\; \rho(m) \le 1 \right\} \\
&= \left\{ \sum_j m_j \phi_j \;:\; \sum_j \lambda_j m_j^2 \le 1 \right\}
\end{aligned}
$$

where ϕ_j and λ_j are the eigenvectors and eigenvalues of the self-adjoint operator $T^\star T$ satisfying $T^\star T u = x u' - u''$.

What are these eigenvectors ϕ_j?

$$
\begin{aligned}
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\end{aligned}
$$

where ϕ_j and λ_j are the eigenvectors and eigenvalues of the self-adjoint operator $T^\star T$ satisfying $T^\star Tu = xu' - u''$.

What are these eigenvectors ϕ_j?

Polynomials. See if you can prove it!

Why Sobolev Models? Why Not?

Advantages

1. In Fourier-series terms, they're familiar.
    - They can help us explain things to people with intro-stats level background.
    - And understand their work better. e.g., we can use them to think about how well we can approximate a smooth function by a polynomial of a given order.
2. They're easy to implement.
    - We don't need clever model-specific tricks to code up and understand things.
    - We did for using Lipschitz or Bounded Variation or Monotone Regression models.
3. They're easy to generalize.
    - It generalizes very naturally to higher order-derivatives. Just change the power of the eigenvalues.
    - We'd have to work a bit harder to generalize our implementation (and understanding) of our other smooth models.

    $$\mathcal{M} = \left\{ m : \int_0^1 |m^{(p)}(x)| dx \le B \right\} \quad \text{The Bounded Variation } (p-1)\text{st Derivative Model}$$

    $$\mathcal{M} = \left\{ m : \max_x |m^{(p)}(x)| \le B \right\} \quad \text{The Lipschitz } (p-1)\text{st Derivative Model}$$

    - The generalization to multi-dimensional covariates is straightforward too. Next week.

Disadvantages

1. It's a bit harder to understand intuitively.
    - I can see from a drawing whether a curve is increasing and whether its derivative is.
    - Or whether it has has small Lipschitz or TV seminorm.
    - With this model, I may have a rough sense, but it's not as easy.
2. Maybe it's not quite what we want.
    - Maybe we know we want a Lipschitz model, e.g. if we're doing RDD.
    - We'd want to ensure it doesn't do anything weird at the data's edge.

Technical Details

Weak Derivatives

A review of orthogonal bases in $\mathbb{R}^n$

- A set of vectors $v_1 \ldots v_n$ is a basis if we can write every vector in $\mathbb{R}^n$ as a *unique* weighted average of the vectors in the basis.

$$\text{for all } v \in \mathbb{R}^n\text{, there exists unique } \alpha \in \mathbb{R}^n \text{ such that } v = \sum_{k=1}^{n} \alpha_k v_k.$$

- A basis is *orthogonal* if all pairs of basis vectors have zero inner product.

$$\langle v_j, v_k \rangle = 0 \quad \text{for} \quad j \neq k.$$

- *Eigenvectors* of a symmetric matrix T are an orthogonal for *two inner products*
  1. The usual inner product, the dot product $\langle u, v \rangle_2$.
  2. An inner product involving T, $\langle u, v \rangle_T = \langle Tu, v \rangle_2$.

  And they form a basis for $\mathbb{R}^n$.

Proving orthogonality of eigenvectors

Orthogonality in the dot product $\langle \cdot, \cdot \rangle_2$

Orthogonality in the inner product $\langle \cdot, \cdot \rangle_T = \langle T \cdot, \cdot \rangle_2$

Proving orthogonality of eigenvectors

Orthogonality in the dot product $\langle \cdot, \cdot \rangle_2$

Let $v_1 \dots v_n$ be eigenvectors of symmetric T with distinct eigenvalues λ_j: $Tv_k = \lambda_k v_k$.

$$\lambda_j \langle v_j, v_k \rangle_2 = \underset{(Tv_j)^T v_k = v_j^T T^T v_k}{\langle Tv_j, v_k \rangle_2} = \underset{v_j^T (T^T v_k) = v_j^T (Tv_k)}{\langle v_j, Tv_k \rangle_2} = \lambda_k \langle v_j, v_k \rangle$$

Because $\lambda_j \neq \lambda_k$, this is true *only if* v_j, v_k are orthogonal in the dot product $\langle \cdot, \cdot \rangle_2$.

Orthogonality in the inner product $\langle \cdot, \cdot \rangle_T = \langle T \cdot, \cdot \rangle_2$

Proving orthogonality of eigenvectors

Orthogonality in the dot product $\langle \cdot, \cdot \rangle_2$

Let $v_1 \dots v_n$ be eigenvectors of symmetric T with distinct eigenvalues λ_j: $Tv_k = \lambda_k v_k$.

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Because $\lambda_j \neq \lambda_k$, this is true *only if* v_j, v_k are orthogonal in the dot product $\langle \cdot, \cdot \rangle_2$.

Orthogonality in the inner product $\langle \cdot, \cdot \rangle_T = \langle T\cdot, \cdot \rangle_2$

$\langle Tv_j, v_k \rangle = \lambda_j \langle v_j, v_k \rangle_2 = 0$ because we have orthogonality in the dot product.

Orthogonal bases for square-integrable functions on $[0, 1]$

- A set of functions $v_1, v_2, \ldots$ is a basis if we can write every square-integrable function on $[0, 1]$ as a *unique* weighted average of the functions in the basis.

  for all $v : \int_0^1 v(x)^2\, dx < \infty$, there exists unique $\alpha_1, \alpha_2, \ldots$ such that $v = \sum_{k=1}^{\infty} \alpha_k v_k$.

- A basis is *orthogonal* if all pairs of basis functions have zero inner product.

$$\langle v_j, v_k \rangle = 0 \quad \text{for} \quad j \neq k.$$

- *Eigenvectors* of a 'symmetric matrix' T are orthogonal for *two inner products*
  1. The usual inner product, $\langle u, v \rangle_{L_2} = \int_0^1 u(x)v(x)\, dx$.
  2. An inner product involving T, $\langle u, v \rangle_T = \langle Tu, v \rangle_{L_2}$.

  And they form a basis, too. Here T is a symmetric matrix if $\langle Tu, v \rangle_{L_2} = \langle u, Tv \rangle_{L_2}$.

Technical Detail

By *a symmetric matrix*, I mean a compact self-adjoint operator.

Theorem (The Spectral Theorem)
Suppose T is a compact self-adjoint operator on a Hilbert space V. Then there is an orthogonal basis of V consisting of eigenvectors of T. Each eigenvalue is real.

The derivative isn't compact, but its inverse is. That turns out to be what matters.