Winter 2021 Math 106
Topics in Applied Mathematics
Data-driven Uncertainty Quantification

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Lecture 11: Smoothing using Orthogonal Functions

11.1 Density estimation using orthogonal functions

- Let $X_1, X_2, ..., X_n$ be IID observations from a distribution on $[0,1]$ with density f. If we assume that $f \in L^2$, we can write

$$f(x) = \sum_{j=0}^{\infty} \beta_j \phi_j(x)$$

  where $\{\phi_j\}$ is an orthonormal basis of $L^2[0,1]$.
- If we know $f(x)$, the coefficient β_j is given by

$$\beta_j = \int_{[0,1]} f(x)\phi_j(x)dx.$$

- The above formula looks similar to the Kernel density estimation. But the basis function $\phi_j(x)$ does not necessarily have measure 1 in contrast to the Kernel.
- Without knowing $f(x)$, how can we calculate the coefficient β_j? We need to estimate it using the data.

11.1 Density estimation using orthogonal functions

- The estimate $\hat{\beta}_j$ of β_j is given by

$$\hat{\beta}_j = \frac{1}{n}\sum_{i}^{n} \phi_j(x_i)$$

Theorem. The mean and variance of $\hat{\beta}_j$ are

$$E[\hat{\beta}_j] = \beta_j, \quad Var(\hat{\beta}_j) = \frac{\sigma_j^2}{n}$$

where $\sigma_j^2 = Var(\phi_j(X_i)) = \int(\phi_j(x) - \beta_j)^2 f(x)dx$.
Proof.

$$E[\hat{\beta}_j] = \frac{1}{n}\sum_{i}^{n} E[\phi_j(X_i)] = E[\phi_j(X_1)) = \int \phi_j(x)f(x)dx = \beta_j.$$

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Exercise. Prove the variance.

11.1 Density estimation using orthogonal functions

- For a given $f(x)$, we know that

$$\sum_{j}^{J} \beta_j \phi_j(x) \tag{1}$$

  is more accurate if $J \in \mathbb{N}$ increases.

- This is not true anymore with the estimates $\{\hat{\beta}_j\}$.
  Think about the regression. A higher order polynomial regression function is not always better than a lower order polynomial regression function (bias and variance tradeoff).
- J is called the **smoothing parameter**. It is typically chosen between 1 and $\sqrt{n}$ where n is the sample size. J is chosen so that it minimizes the **risk** (or **mean integrated squared error**).

11.1 Density estimation using orthogonal functions

Let $\hat{f}(x)$ is an estimate of $f(x)$ given by

$$\hat{f}(x) = \sum_{j}^{J} \hat{\beta}_j \phi_j(x).$$

Remember that the risk of $\hat{f}$ using a smoothing parameter J is the expected value of the L^2 error, that is

$$R(J) = E\left[\int (\hat{f}(x) - f(x))^2 dx\right] = \sum_{j=1}^{J} \frac{\sigma_j^2}{n} + \sum_{j=J+1}^{\infty} \beta_j^2.$$

11.1 Density estimation using orthogonal functions

Theorem. An estimate of the risk $R(J)$ is

$$\hat{R}(J) = \sum_{j=1}^{J} \frac{\hat{\sigma}_j^2}{n} + \sum_{j=J+1}^{\infty} \left(\hat{\beta}_j^2 - \frac{\hat{\sigma}_j^2}{n} \right)_+$$

where $a_+ = \max\{a, 0\}$ and

$$\hat{a}_j^2 = \frac{1}{n-1} \sum_{i}^{n} \left(\phi_j(X_i) - \hat{\beta}_j \right)^2 .$$

- Using the J^* that minimizes $\hat{R}(J)$, the estimate of the density $\hat{f}(x)$ is given by
$$\hat{f}(x) = \sum_{j}^{J^*} \hat{\beta}_j \phi_j(x)$$
- Note that $\hat{f}(x)$ can be negative!! If so, take $\hat{f}^* = \max(\hat{f}, 0)$ and normalize it.

11.2 Regression

For a data set $\{X_i, Y_i\}$,

- Remember that the regression function $r(x)$ is defined as the expected value of Y given x

$$r(x) = E[Y|X = x].$$

- We studied parametric and nonparametric regressions. In particular, for nonparametric regression, we know a kernel density estimation based regression method.
- It is also possible to calculate a regression function using density estimation with orthogonal functions.
- Assume that $r(x)$ is in $L^2(0,1)$ and x_i is uniformly distributed.
- $r(x) = \sum_{j=1}^{\infty} \beta_j \phi_j(x)$ where $\beta_j = \int_0^1 r(x)\phi_j(x)dx$ for an orthonormal basis $\{\phi_j\}$ of $L^2(0,1)$.

11.2 Regression

- The estimate of β_j, $\hat{\beta}_j$ is given by

$$\hat{\beta}_j = \frac{1}{n}\sum_{i=1}^{n} Y_i \phi_j(x_i), \quad j = 1, 2, ...$$

Theorem.

$$\hat{\beta}_j \sim N(\beta_j, \frac{\sigma^2}{n})$$

where σ^2 is the variance of the measurement error e_i

$$Y_i = r(x_i) + e_i$$

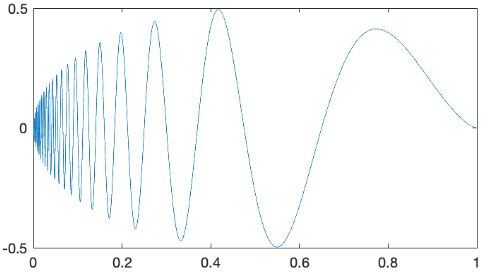
Idea of Proof. For the mean,

$$E[\hat{\beta}_j] = \frac{1}{n}\sum_{i=1}^{n} E[Y_i]\phi_j(x_i) = \frac{1}{n}\sum_{i=1}^{n} r(x_i)\phi_j(x_i)$$

$$\sim \int r(x)\phi_j(x)dx = \beta_j.$$

11.3 Wavelets

- Suppose that a regression function $r(x)$ has a sharp jump but that $r(x)$ is otherwise very smooth. That is, $r(x)$ is spatially inhomogeneous.
- Doppler function $\sqrt{x(1-x)}\sin\left(\frac{2.1\pi}{x+.05}\right)$



11.3 Wavelets

Wavelets are local orthogonal functions.

Harr wavelet.

- Harr father wavelet (or Harr scaling function)

$$\phi(x) = \begin{cases} 1 & \text{if } 0 \leq x < 1 \\ 0 & \textit{otherwise}. \end{cases}$$

- Haar mother wavelet

$$\psi(x) = \begin{cases} -1 & \text{if } 0 \leq x \leq 1/2 \\ 1 & \text{if } 1/2 < x \leq 1 \end{cases}$$

- For any integers j and k define

$$\psi_{j,k}(x) = 2^{j/2}\psi(2^j x - k).$$

- Let $W_j = \{\psi_{jk}, k = 1, 2, ..., 2^j - 1\}$ be the set of rescaled and shifted mother wavelets at resolution j.

11.3 Wavelets

Theorem. The set of functions

$$\{\phi, W_0, W_1, ...\}$$

is an orthonormal basis for $L^2(0,1)$.

Corollary. For any $f \in L^2(0,1)$,

$$f(x) = \alpha\phi(x) + \sum_{j}^{\infty} \sum_{k=0}^{2^j-1} \beta_{j,k}\psi_{j,k}(x)$$

where $\alpha = \int_0^1 f(x)\phi(x)dx$, $\beta_{j,k} = \int_0^1 f(x)\psi_{j,k}(x)dx$.

- α is called **scaling coefficient**.
- $\beta_{j,k}$ are called **detail coefficients**.
- In a finite sum approximation of f using J different scales

$$f(x) = \alpha\phi(x) + \sum_{j}^{J} \sum_{k=0}^{2^j-1} \beta_{j,k}\psi_{j,k}(x)$$

J represents the resolution of the approximation.

11.3 Wavelets

Regression.

- Consider the regression model $Y_i = r(x_i) + \sigma e_i$ where $e \sim N(0, 1)$ and $x_i = i/n$.
- For simplicity, assume that $n = 2^J$ for some J.
- Smoothing with wavelets requires thresholding instead of truncation. That is, instead of choosing a smoothing parameter that determines the number of terms to keep, thresholding keeps coefficients that are sufficiently large.
- One example of thresholding is **hard**, **universal** thresholding.

11.3 Wavelets

Hard, universal thresholding.

1. Calculate

$$\hat{\alpha} = \frac{1}{n} \sum_i \phi_k(x_i) Y_i, \quad \text{and} \quad D_{j,k} = \frac{1}{n} \sum_k \psi_{j,k}(x_i) Y_i$$

   for $0 \leq j \leq J-1$ where $J = \log_2(n)$.

2. Apply universal thresholding

$$\hat{\beta}_{j,k} = \begin{cases} D_{j,k} & \text{if } |D_{j,k}| > \text{threshold value} \\ 0 & \text{otherwise} \end{cases}$$

3. Set $\hat{r}(x) = \hat{\alpha}\phi(x) + \sum_{j=0}^{J-1} \sum_{k=0}^{2^j-1} \hat{b}_{j,k} \psi_{j,k}(x)$.

Homework

For $n = 10,000$, set $x_i = i/n$ and $y_i = \text{doppler}(x_i) + e_i$ where $e_i \sim N(0, 0.05^2)$.

1. Use the trigonometric functions to estimate the regression function.
2. Use the Legendre polynomials to estimate the regression function.
3. Use the Harr wavelets to estimate the regression function.

For 1-3, try to use a small number of terms. You are okay to use any programming libraries (that is, you do not need to make your own code; just use standard libraries) but specify all parameters to get your estimates.