Lecture 4: Basis Expansions, Local Averaging & Kernel Smoothing

Readings: ESL (Ch. 5.1-5.6, 6), ISL (Ch. 7), Bach (Ch. 6); code

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September 4, 2025

Outline

1. Global Methods: Basis Expansions
2. Regression Splines
3. Smoothing Splines
4. Local Methods: Averaging & Kernels
5. Kernel Smoothing Methods
6. Kernel Density Estimation
7. The Kernel Density Classifier
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The Core Idea of Basis Expansions

Make linear models more flexible by augmenting/replacing the inputs X with a pre-specified set of transformations, or **basis functions**, $h_m(X) : \mathbb{R}^p \to \mathbb{R}$.

Definition 1: Linear Basis Model

The model takes the general form:

$$f(X) = \sum_{m=1}^{M} \beta_m h_m(X). \quad (h_M = \text{feature map})$$

- The function $f(X)$ is now a flexible, nonlinear function of the input X.
- The model is still a **linear** model with respect to the coefficients β_m.
- The ERM problem is easy: We can use all the machinery of linear models (OLS, ridge, or lasso) on the new "predictor" matrix $\mathbf{H}$, $\mathbf{H}_{im} = h_m(x_i)$.

This is a **global method**: the value of the prediction function at any point x depends on all of the β_m, which in turn depend on all of the training data.

Piecewise Polynomials

Assume $X \in \mathbb{R}$ ($p = 1$) from now on for simplicity.

Definition 2: Piecewise Polynomial

Divide the domain of X into contiguous intervals and represent f by a separate polynomial in each interval.

The simplest case: piecewise constants (step functions)

$$f(X) = \sum_{m=0}^{M} c_m I(X \in C_m)$$

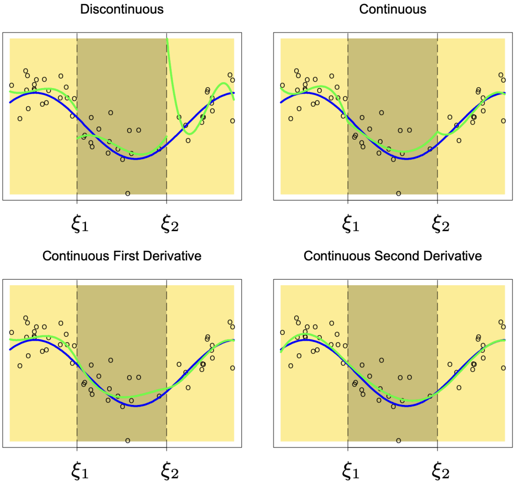
where C_m are disjoint regions covering $\mathbb{R}$.

- Unless constrained to be continuous, they can jump at the boundaries
- Discontinuities may not be desirable for regression
- Need to address smoothness at the knots

💡 **Solution:** Impose continuity constraints at the boundary points (knots) ξ_j.

Why Smoother Functions are Preferred

A series of piecewise-cubic polynomials fit to data (see ESL Ch. 5.2):



Piecewise Polynomials and Splines

Definition 3: Order-M Spline

An order-M spline with knots $\xi_j, j = 1, \ldots, K$ is a piecewise-polynomial of order M, and has continuous derivatives up to order $M - 2$.

A cubic spline (order 4) has continuous first and second derivatives at each knot.

The Truncated Power Basis

A cubic spline with K knots can be represented by a basis of $K + 4$ functions:

$$h_1(X) = 1,\ h_2(X) = X,\ h_3(X) = X^2,\ h_4(X) = X^3,$$

$$h_{j+4}(X) = (X - \xi_j)_+^3, \quad j = 1, \ldots, K$$

where $(z)_+ = \max(0, z)$ is the positive part function.

Key insight: The truncated power functions $(X - \xi_j)_+^3$ are zero to the left of ξ_j and behave like $(X - \xi_j)^3$ to the right, allowing for smooth joins.

Natural Cubic Splines

Definition 4: Natural Cubic Spline

A natural cubic spline adds the constraint that the function is linear beyond the boundary knots.

Motivation: The behavior of polynomials fit to data is notoriously bad at the boundaries. The linear constraint prevents wild extrapolation.

Basis for Natural Cubic Splines. For knots $\xi_1 < \xi_2 < \ldots < \xi_K$, the K basis functions are:

$$N_1(X) = 1, \quad N_2(X) = X, \tag{1}$$

$$N_{j+2}(X) = d_j(X) - d_{K-1}(X), \quad j = 1, \ldots, K-2, \tag{2}$$

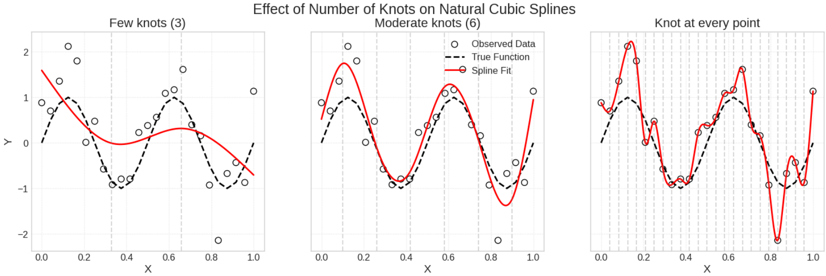
where

$$d_j(X) = \frac{(X - \xi_j)_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_j}.$$

Natural cubic splines often give superior fits at the boundaries.

Natural Cubic Splines: How to choose K?

- We generate noisy observations from the function $y = \sin(4\pi x)$.
- We fit **natural cubic splines** with different numbers of knots:
  - **Few knots (3):** The spline is very smooth and underfits the oscillations.
  - **Moderate knots (6):** The spline balances smoothness and flexibility, capturing the main trend.
  - **Knot at every data point:** The spline interpolates almost exactly, leading to overfitting.



B-Splines

Truncated power basis is numerically unstable for large numbers of knots. B-splines provide a basis with better numerical properties.

Definition 5: B-Spline Basis

Each basis function $B_{i,m}(x)$ has local support over at most $m+1$ knots.

Properties of B-Splines

- $B_{i,m}(x) \geq 0$ for all i, m, x.
- $B_{i,m}(x) = 0$ unless $\xi_i \leq x \leq \xi_{i+m+1}$ (local support).
- $\sum_i B_{i,m}(x) = 1$ for all x (partition of unity).
- They have the smallest support among all positive spline bases.

Computation: B-splines can be computed efficiently using the stable recurrence relations of de Boor (1978).

Advantage: Changing one coefficient affects the spline function only locally.

Smoothing Splines

Different approach: Instead of fixing the knots in advance, use the maximal set of knots and control the function's smoothness by regularization.

Definition 6: Smoothing Spline

Among all functions f with two continuous derivatives, find the one that minimizes the penalized residual sum of squares:

$$\text{PRSS}(f, \lambda) = \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \int f''(t)^2 dt$$

where $\lambda \geq 0$ is a fixed smoothing parameter.

- The first term measures closeness to the data.
- The second term is a **roughness penalty**. It measures the total curvature of the function.
- The smoothing parameter controls the bias-variance trade-off.

Solution

Theorem 1: Solution to Smoothing Spline Problem

The minimizer of $\text{PRSS}(f, \lambda)$ is a natural cubic spline with knots at the unique values of the x_i, $i = 1, 2, \ldots, N$.

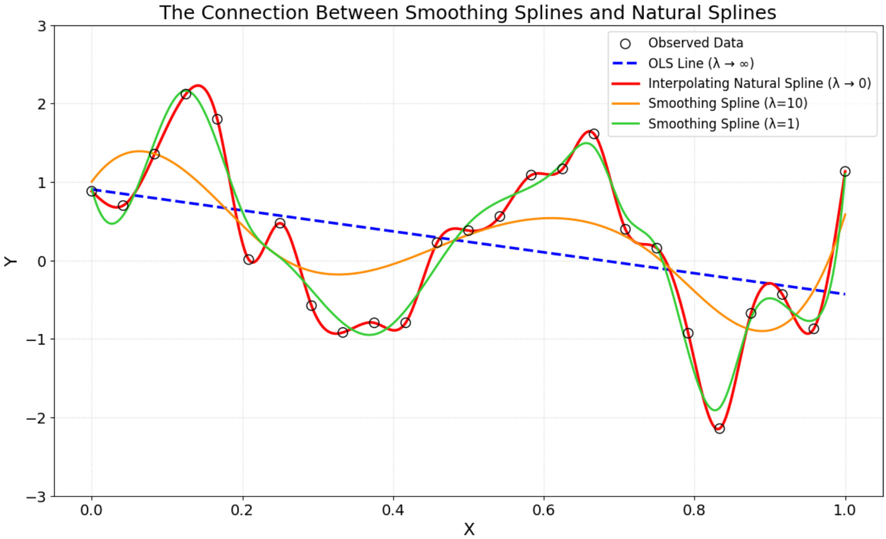
Proof.

See Exercise 5.1. □

Key points:

- $\lambda = 0$: interpolating spline (overfitting)
- $\lambda = \infty$: linear least squares fit
- The solution is a finite-dimensional natural spline despite the infinite-dimensional optimization.

Illustration (Using the Same Data As Before)



Matrix Formulation of Smoothing Splines

Let $\mathbf{N}$ be the $N \times N$ matrix of natural spline basis functions evaluated at the training points x_i.

Matrix Form: The smoothing spline can be written as

$$\hat{f}(x) = \sum_{j=1}^{N} N_j(x)\theta_j$$

where $\boldsymbol{\theta} = (\mathbf{N}^T\mathbf{N} + \lambda\boldsymbol{\Omega}_N)^{-1}\mathbf{N}^T\mathbf{y}$ and $(\boldsymbol{\Omega}_N)_{jk} = \int N_j''(t)N_k''(t)dt$.

The fitted values are given by:

$$\hat{\mathbf{y}} = \mathbf{N}(\mathbf{N}^T\mathbf{N} + \lambda\boldsymbol{\Omega}_N)^{-1}\mathbf{N}^T\mathbf{y} = \mathbf{S}_\lambda\mathbf{y}$$

where $\mathbf{S}_\lambda$ is the **smoother matrix**.

Properties and Effective Degrees of Freedom

Proposition 1: Properties of Smoother Matrix

$\mathbf{S}_\lambda$ is symmetric and positive semi-definite with eigenvalues in $[0, 1]$.

Proof.

See blackboard. □

Intuition: The effective degrees of freedom $\mathrm{df}_\lambda = tr(\mathbf{S}_\lambda)$ measures the effective number of parameters in the smoothing spline fit.

- $\lambda = 0$: $\mathrm{df}_\lambda = N$ (interpolating spline)
- $\lambda \to \infty$: $\mathrm{df}_\lambda = 2$ (linear fit)

💡 We can write $\mathbf{S}_\lambda$ in the Reinsch form $\mathbf{S}_\lambda = (\mathbf{I} + \lambda \mathbf{K})^{-1}$, where $\mathbf{K}$ does not depend on λ (see Exercise 4.1-4.2) and is known as the penalty matrix since $\hat{\mathbf{f}} = \mathbf{S}_\lambda \mathbf{y}$ solves

$$\min_{\mathbf{f}} (\mathbf{y} - \mathbf{f})^T (\mathbf{y} - \mathbf{f}) + \lambda \mathbf{f}^T \mathbf{K} \mathbf{f}.$$

From Global to Local Methods

Instead of fitting a single global function, we can compute a separate fit at each target point x_0 using only the training data that is **local** to that point.

Definition 7: Local Averaging Estimators

A local averaging estimator has the general form: $\hat{f}(x_0) = \sum_{i=1}^{N} w_i(x_0) y_i$ where the weights $w_i(x_0)$ depend on the target point x_0.

- **Nearest Neighbors:** The weights are $w_i(x_0) = \frac{1}{k}$ if x_i is one of the k nearest neighbors of x_0, and 0 otherwise.
- **Kernel Smoothing:** The weights are defined by a kernel function that smoothly down-weights points as their distance from x_0 increases.

Smoothing Splines are Kernel Smoothers

- The smoother matrix $\mathbf{S}_\lambda$ defines a set of weights for each target point. The prediction at a point x_i is a weighted average of all y_j.
- For any linear smoother $\mathbf{S}$, the prediction at a point x_0 can be written as a locally weighted average:

  $$\hat{f}(x_0) = \sum_{i=1}^{N} L(x_0, x_i) y_i$$

  The function $L(x_0, \cdot)$ is called the **equivalent kernel** of the smoother.
- The smoothing spline, which we derived from a global, penalized regression problem, is in fact a kernel smoother. Its equivalent kernel is locally adaptive—the bandwidth of the kernel is wider in regions where the data is more sparse.
- A penalized global basis expansion in the primal space can be equivalent to a local kernel smoother in the dual space. This idea is central to the theory of SVMs and other kernel methods.

One-Dimensional Kernel Smoothers

Definition 8: The Nadaraya-Watson Kernel Estimator

The prediction at a point x_0 is a weighted average of the observed y_i:

$$\hat{f}(x_0) = \frac{\sum_{i=1}^{N} K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^{N} K_\lambda(x_0, x_i)}$$

where $K_\lambda(x_0, x) = \frac{1}{\lambda} K\left(\frac{|x - x_0|}{\lambda}\right)$ is a kernel function with bandwidth λ.

Common Kernel Functions (typically symmetric, non-negative function that integrates to one):

Epanechnikov: $K(t) = \frac{3}{4}(1 - t^2)$ if $|t| \leq 1$, 0 otherwise (see Exercise 4.3)
Tri-Cube: $K(t) = (1 - |t|^3)^3$ if $|t| \leq 1$, 0 otherwise
Gaussian: $K(t) = \phi(t)$ where ϕ is standard normal density

💡 The Epanechnikov kernel is optimal in a mean-squared error sense, though the choice of kernel is generally less important than the choice of bandwidth λ.

Local Polynomial Regression: Correcting Boundary Bias

The Nadaraya-Watson estimator, which fits a local constant, suffers from significant bias at the boundaries of the data. This is because its averaging window becomes one-sided.

Definition 9: Local Polynomial Regression

Instead of a local constant, we fit a local polynomial model at each target point x_0 by solving a weighted least squares problem:

$$\min_{\beta(x_0)} \sum_{i=1}^{N} K_\lambda(x_0, x_i) \left(y_i - \sum_{j=0}^{d} \beta_j(x_0)(x_i - x_0)^j \right)^2$$

The fit is the constant term of the local polynomial: $\hat{f}(x_0) = \hat{\beta}_0(x_0)$.

The most important case is local linear regression.

Local Linear Regression

Definition 10: Local Linear Regression

At each target point x_0, solve:

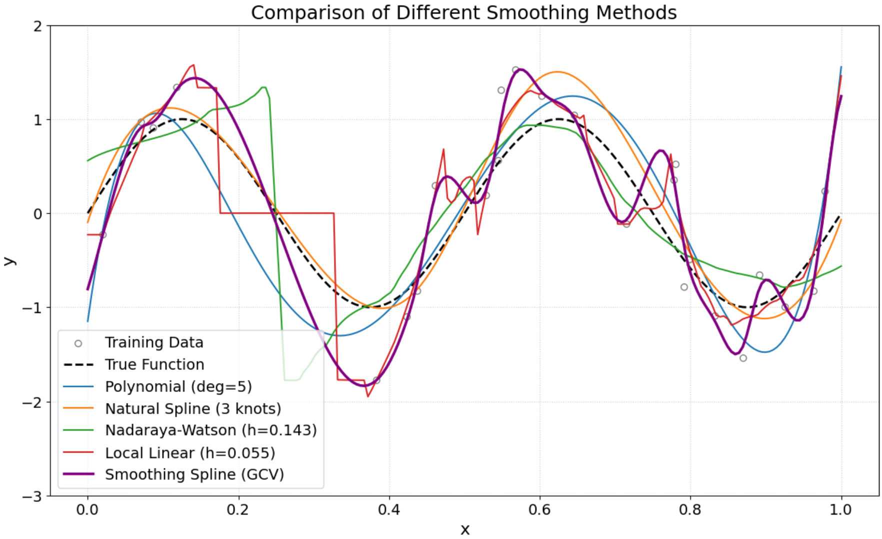
$$\min_{\alpha,\beta} \sum_{i=1}^{N} K_\lambda(x_0, x_i)[y_i - \alpha - \beta(x_i - x_0)]^2.$$

The estimate is $\hat{f}(x_0) = \hat{\alpha}$.

Matrix form: The local linear estimate can be written as $\hat{f}(x_0) = \mathbf{l}(x_0)^T \mathbf{y}$ where $\mathbf{l}(x_0)$ are the equivalent kernel weights.

- Nadaraya-Watson has bias of order $O(h^2)$ in the interior but $O(h)$ at boundaries (local linear regression has bias of order $O(h^2)$ everywhere, including boundaries).
- Local linear regression automatically adapts to local slope.

Comparison Demo (Using The Same Data As Before)



Asymptotic Bias and Variance of Kernel Smoothers

Assume $y = f(x) + \varepsilon$ where $\mathbb{E}[\varepsilon] = 0$ and $\mathrm{Var}(\varepsilon) = \sigma^2$. For a test point x_0,

$$\mathrm{MSE}(\hat{f}(x_0)) = (\mathbb{E}[\hat{f}(x_0)] - f(x_0))^2 + \mathrm{Var}(\hat{f}(x_0)) = \text{squared bias} + \text{variance}.$$

Let $\hat{f}$ be the Nadaraya-Watson kernel estimator with bandwidth h. Assume:

- The training points x_i are a fixed design with density $p(x)$.
- The true function $f(x)$ is twice continuously differentiable.
- The kernel $K(u)$ is a symmetric probability density with $\int uK(u)du = 0$.
- As $N \to \infty$, we have $h \to 0$ and $Nh \to \infty$.

Then, the leading terms for the bias and variance at x_0 are:

- $\mathrm{Bias}^2(\hat{f}(x_0)) \approx \left[\frac{h^2}{2}\left(f''(x_0) + \frac{2f'(x_0)p'(x_0)}{p(x_0)}\right)\int u^2 K(u)du\right]^2 = O(h^4)$.
- $\mathrm{Var}(\hat{f}(x_0)) \approx \frac{\sigma^2}{Nhp(x_0)}\int K(u)^2 du = O\left(\frac{1}{Nh}\right)$.

💡 Minimizing $h^4 \cdot C_1 + \frac{1}{Nh} \cdot C_2$ with respect to h shows that the optimal bandwidth is of order $N^{-1/5}$. This yields optimal error rate of $\boldsymbol{O(N^{-4/5})}$.

Local Regression in Higher Dimensions

Definition 11: Multivariate Local Linear Regression

At each target point $x_0 \in \mathbb{R}^p$, solve the weighted LS problem:

$$\min_{\beta_0, \boldsymbol{\beta}} \sum_{i=1}^{N} K_\lambda(x_0, x_i)[y_i - \beta_0 - \boldsymbol{\beta}^T(x_i - x_0)]^2$$

where $K_\lambda(x_0, x) = \frac{1}{\lambda^p} K\left(\frac{\|x - x_0\|}{\lambda}\right)$.

Let $\mathbf{B}$ be the $N \times (p+1)$ regression matrix with i-th row $b(x_i)^T = (1, x_i - x_0)$. Let $\mathbf{W}(x_0)$ be the $N \times N$ diagonal weight matrix with $W_{ii} = K_\lambda(x_0, x_i)$. Then: $\hat{\boldsymbol{\theta}} = (\mathbf{B}^T\mathbf{W}(x_0)\mathbf{B})^{-1}\mathbf{B}^T\mathbf{W}(x_0)\mathbf{y}$, and the fit is $\hat{f}(x_0) = b(x_0)^T\hat{\boldsymbol{\theta}} = l(x_0)^T\mathbf{y}$.

Curse of dimensionality: The radius of a neighborhood containing a fixed fraction of the data grows like $N^{-1/p}$, so local neighborhoods become less local as p increases.

Structured Models in $\mathbb{R}^p$

Local regression in high dimensions requires enormous datasets to work well.
Solution: Impose structure to avoid the curse of dimensionality.

Definition 12: Structured Local Regression

Instead of using all p dimensions, use a structured model like:

- **Varying coefficient model:** $f(X) = \alpha(X_1) + \beta(X_1)X_2$
- **Additive model:** $f(X) = \sum_{j=1}^{p} f_j(X_j)$

Locally Weighted Running Line Smoother (LOWESS) is a robust version that:

1. Performs local linear regression.
2. Computes residuals and assigns weights based on their size.
3. Re-fits using these robustness weights.
4. Iterates until convergence.

This provides resistance to outliers in the data.

Kernel Density Estimation

Definition 13: Kernel Density Estimator (KDE)

Given i.i.d. sample $x_1, \ldots, x_N$ from density $f(x)$:

$$\hat{f}(x) = \frac{1}{N\lambda} \sum_{i=1}^{N} K\left(\frac{x - x_i}{\lambda}\right)$$

where K is a probability density function.

- $\hat{f}(x) \geq 0$ and $\int \hat{f}(x)dx = 1$.
- $\mathbb{E}[\hat{f}(x)] = (K * f)(x)$ (convolution with scaled kernel).
- As $\lambda \to 0$ and $N\lambda \to \infty$: $\hat{f}(x) \to f(x)$ pointwise.
- **Connection to Nadaraya-Watson estimator:** See Exercise 4.4.
- **Naive Bayes classification via KDE**: Estimate class densities via $\hat{f}_k(x) = \frac{1}{N_k\lambda} \sum_{x_i \in C_k} K\left(\frac{x-x_i}{\lambda}\right)$. Classify using: $\hat{G}(x) = \arg\max_k \hat{\pi}_k \hat{f}_k(x)$, where $\hat{\pi}_k = N_k/N$.

Radial Basis Functions (RBF)

Definition 14: Radial Basis Function Expansion

$$f(x) = \sum_{m=1}^{M} K_{\lambda_m}(\mu_m, x)\beta_m,$$

where $K_{\lambda_m}(\mu_m, \cdot)$ is a kernel function centered at μ_m with scale parameter λ_m.

Gaussian RBF network is a popular choice: $K_\lambda(\mu, x) = e^{-\frac{\|x-\mu\|^2}{2\lambda^2}}$, with the resulting $f(x)$ having the parameters:

- Centers μ_m (often chosen as subset of training points)
- Scales λ_m (often kept constant)
- Coefficients β_m (via least squares)

Key difference from kernel methods: M is typically much smaller than N.
Connection to neural networks: RBF networks are a type of neural network with one hidden layer, but with radial basis activation functions instead of sigmoids.

Selecting the Width of the Kernel

The bias-variance tradeoff:

- Small λ: low bias, high variance (undersmoothing)
- Large λ: high bias, low variance (oversmoothing)

Definition 15: Cross-Validation for Bandwidth Selection

Choose λ to minimize:

$$\mathrm{CV}(\lambda) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{f}_{-i}(x_i))^2$$

where $\hat{f}_{-i}$ is the estimate with the i-th observation removed.

💡 Efficient CV computation for Nadaraya-Watson estimator:

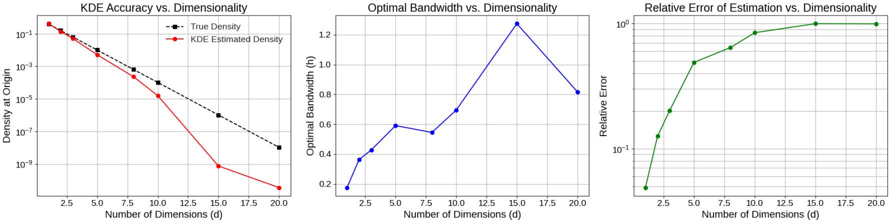
$$y_i - \hat{f}_{-i}(x_i) = \frac{y_i - \hat{f}(x_i)}{1 - S_{ii}(\lambda)}$$

where $S_{ii}(\lambda)$ is the i-th diagonal element of the smoother matrix. This allows CV computation with a single fit instead of N separate fits.

Curse of Dimensionality

Generate 2000 data points from the standard multivariate Gaussian and use KDE to estimate the PDF at the origin (mode of the distribution).

The Curse of Dimensionality for KDE (N = 2000 samples)



⚠ **Over-estimation:** The KDE estimator is forced to select a huge bandwidth in high dimensions, reporting a smeared-out average over a large, non-local region.

Kernel Density Classification

Recall: The goal of classification is to estimate the probability that an observation X belongs to class k.

$$P(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

- $P(Y = k|X = x)$: The posterior probability — what we want.
- $\pi_k = P(Y = k)$: The prior probability of class k.
- $f_k(x) = p(x|Y = k)$: The class-conditional probability density.

The Optimal Decision Rule: Assign x to the class k that maximizes the numerator:

$$\text{Class}(x) = \underset{k}{\operatorname{argmax}} \left(\pi_k f_k(x)\right)$$

The Core Challenge: Estimating the Density $f_k(x)$

The Bayes rule is perfect, but in practice, we never know the true class-conditional densities $f_k(x)$. We must estimate them from the training data.

1. **Parametric Methods**
   - Assume a specific functional form for $f_k(x)$ (e.g., a Multivariate Gaussian).
   - Example: Linear Discriminant Analysis (LDA).
   - **Pro:** Efficient if assumptions are correct.
   - **Con:** High bias; performs poorly if assumptions are violated.

2. **Non-Parametric Methods**
   - Do not assume a specific form for $f_k(x)$. Let the data speak for itself.
   - Example: **Kernel Density Estimation (KDE).**
   - **Pro:** Highly flexible; can capture complex density shapes.
   - **Con:** Requires more data; can be computationally intensive.

The General Kernel Density Classifier

This is the most direct non-parametric approach.

1. **Split Data:** Divide the training data by class $(C_1, C_2, \dots, C_K)$.
2. **Estimate Priors:** Estimate $\hat{\pi}_k$ as the proportion of samples in class k. $(\hat{\pi}_k = N_k/N)$.
3. **Estimate Densities:** For each class k, use Kernel Density Estimation on the data in C_k to get an estimate $\hat{f}_k(x)$.
4. **Classify:** For a new point x_{new}, apply the Bayes rule using these estimates:

$$\text{Class}(x_{new}) = \underset{k}{\text{argmax}} \left(\hat{\pi}_k \hat{f}_k(x_{new}) \right).$$

⚠ This works well in low dimensions (1 or 2). But estimating the *joint* multivariate density $\hat{f}_k(x)$ with KDE suffers severely from the **Curse of Dimensionality**.

The Solution: The Naive Bayes Assumption

To overcome the curse of dimensionality, assume that within each class, the features are independent of one another. This allows us to factorize the joint class-conditional density $f_k(x)$ into a product of one-dimensional marginal densities:

$$f_k(x) = f_k(x_1, x_2, \ldots, x_p) = \prod_{j=1}^{p} f_{kj}(x_j)$$

where $f_{kj}(x_j)$ is the density of the j-th feature for an observation from class k.

Why is this "Naive"?

- In most real-world problems, features are not truly independent (e.g., height and weight are correlated).
- However, the assumption often works remarkably well in practice and makes the problem tractable.

The Naive Bayes Classifier with KDE

Combines the flexibility of KDE with the dimensionality-reducing power of the Naive Bayes assumption.

1. **Estimate Priors:** As before, $\hat{\pi}_k = N_k/N$.
2. **Estimate Marginal Densities:**
   - For **each class k** and for **each feature j**:
   - Use the data from class k and feature j to build a 1-dimensional KDE, giving you $\hat{f}_{kj}(x_j)$.
3. **Combine Densities:** The full class-conditional density estimate is:

$$\hat{f}_k(x) = \prod_{j=1}^{p} \hat{f}_{kj}(x_j).$$

4. **Classify:** Apply the Bayes rule with this factorized form:

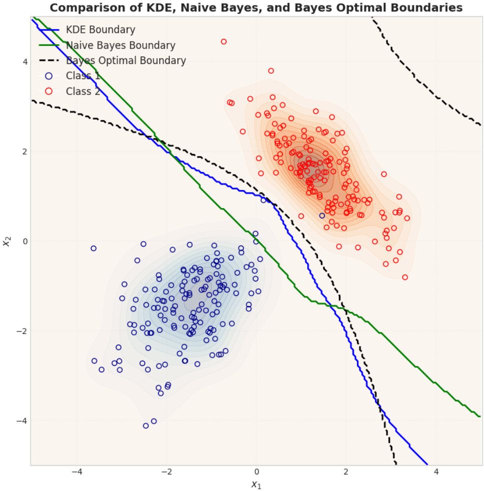
$$\text{Class}(x_{new}) = \underset{k}{\operatorname{argmax}} \left(\hat{\pi}_k \prod_{j=1}^{p} \hat{f}_{kj}(x_{new,j}) \right).$$

**In practice, we compute the sum of log-probabilities to avoid numerical underflow.*

Effect of the Independence Assumption in Naive Bayes

Two classes of 2D data, sample 150 samples from each for training.

Class 1: $X \sim \mathcal{N}([-1.5, -1.5], \begin{bmatrix} 0.8 & 0.4 \\ 0.4 & 0.8 \end{bmatrix})$; Class 2: $X \sim \mathcal{N}([1.5, 1.5], \begin{bmatrix} 0.8 & -0.6 \\ -0.6 & 0.8 \end{bmatrix})$.



Exercises

Exercise 4

1. Solve Exercise 5.7 in ESL.
2. Solve Exercise 5.9 and 5.11 in ESL.
3. Verify that the Epanechnikov kernel function is a symmetric probability distribution function and solve Exercise 6.1 in ESL.
4. Solve Exercise 6.8 in ESL.
5. **Analysis of Linear Kernel Smoothers in the Fixed Design Setting.** Solve Exercise 6.10 in ESL.

Exercises

Exercise 4 (Experimental)

Generate a simple one-dimensional dataset with $N = 50$ points from the model: $y = \sin(2\pi x^3) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, 0.2^2)$, where x is drawn uniformly from $[0, 1]$.

- Fit a global polynomial of degree 5.
- Fit a natural cubic spline with knots placed at the 25th, 50th, and 75th percentiles of the data.
- Fit a Nadaraya-Watson (local constant) kernel smoother.
- Fit a local linear kernel smoother.
- Fit a smoothing spline.

For the above methods, use 5-fold CV to select the optimal bandwidth or effective degrees of freedom. Plot all five fitted curves on top of the training data and the true function. Discuss the results.

Appendix: Derivation of Asymptotic Bias and Variance

The derivation requires approximating discrete sums with integrals. This is only valid under the assumption that as $N \to \infty$, we have $h \to 0$ and $Nh \to \infty$. The expected value is $\mathbb{E}[\hat{f}(x_0)] = \frac{\sum_{i=1}^{N} K_h(x_0, x_i) f(x_i)}{\sum_{j=1}^{N} K_h(x_0, x_j)}$.

Step 1: Taylor Expansion. We expand $f(x_i)$ around x_0. This is only accurate if $|x_i - x_0|$ is small. Since the kernel's support is of width h, we require $\boldsymbol{h \to 0}$.

$$f(x_i) \approx f(x_0) + (x_i - x_0) f'(x_0) + \frac{(x_i - x_0)^2}{2} f''(x_0)$$

Step 2: Approximate Sums with Integrals. This step is valid because the number of points in the kernel's window is large, which requires $\boldsymbol{Nh \to \infty}$. Let $u = (x - x_0)/h$.

$$\text{Denominator} = \sum_j K_h(x_j, x_0) \approx N \int K\left(\frac{x - x_0}{h}\right) p(x) dx = Nh \int K(u) p(x_0 + hu) du \approx Nhp(x_0)$$

Step 3: Combine and Solve. Applying the same steps to the numerator and using the symmetry of the kernel (so terms with odd powers of u vanish), the leading bias term is:
$\text{Bias}(\hat{f}(x_0)) \approx \frac{h^2}{2} f''(x_0) \int u^2 K(u) du$.
The variance is $\text{Var}(\hat{f}(x_0)) = \sigma^2 \frac{\sum_i K_h(x_0, x_i)^2}{(\sum_j K_h(x_0, x_j))^2}$. Again, we approximate the sums with integrals, which requires $\boldsymbol{Nh \to \infty}$:

$$\text{Numerator Sum} \approx N \int K\left(\frac{x - x_0}{h}\right)^2 p(x) dx \approx Nhp(x_0) \int K(u)^2 du$$

$$\text{Denominator Sum}^2 \approx (Nhp(x_0))^2$$

Combining these gives the final result: $\text{Var}(\hat{f}(x_0)) \approx \sigma^2 \frac{Nhp(x_0) \int K(u)^2 du}{(Nhp(x_0))^2} = \frac{\sigma^2}{Nhp(x_0)} \int K(u)^2 du$.