Module 2: Spline and Kernel Methods

Spline and Kernel Methods for GLMs

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Review of GLMs

- Mean parameters are a linear combination of inputs, passed through a possibly nonlinear function
- Assume a distribution in the exponential family

natural param   log-partition fcn   Focus on canonical form

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + \underbrace{c(y, \sigma^2)}\right]$$

dispersion   const. wrt θ

  - Using theory of exponential families,

$$\mu(x) = E[Y \mid x] = b'(\theta(x))$$

$$\mathrm{var}(Y \mid x) = \sigma^2 b''(\theta(x)) \triangleq \sigma^2 V_x$$

Review of GLMs

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Mean parameters are a linear combination of inputs, passed through a possibly nonlinear function
- A parametric GLM assumes

$$\underbrace{g}_{\text{"link fcn"}}(\mu(x)) = \beta^T x$$

  - With a canonical link function,

$$\theta(x) = g(\mu(x))$$

  - The link function is assumed to be invertible

$$\mu(x) = g^{-1}(\theta(x))$$

Examples

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Linear regression

$\theta_i = \theta(x_i)$ $\quad$ $b(\theta)$

$$\log p(y_i \mid x_i, \beta, \sigma^2) = \frac{y_i \tilde{\mu}_i - \frac{\tilde{\mu}_i^2}{2}}{\sigma^2} \underbrace{- \frac{1}{2}\left(\frac{y_i^2}{\sigma^2} + \log(2\pi\sigma^2)\right)}_{c(y_i, \sigma^2)}$$

$\theta_i = \tilde{\mu}_i = \beta^T x_i$

$b(\theta(x)) = \frac{\theta(x)^2}{2}$

$\mu(x) = b'(\theta(x)) = \theta(x) = \tilde{\mu}(x)$

$b''(\theta) = 1 \Rightarrow var(y_i) = \sigma^2 b''(\theta) = \sigma^2$

$\theta(x) = g(\mu(x))$

$= \tilde{\mu}(x) = \mu(x)$

$\Rightarrow g(\cdot) = I(\cdot)$

$g(t) = t$ Identity link fcn

Examples

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Binomial regression

$$\log p(y_i \mid x_i, \beta, \sigma^2) = \overbrace{y_i \log\left(\frac{\pi_i}{1-\pi_i}\right)}^{\theta_i} + \overbrace{m \log(1-\pi_i)}^{-b(\theta)} + \overbrace{\log\binom{m}{y_i}}^{c}$$

$\sigma^2 = 1$

$\theta(x) = \log \frac{\pi(x)}{1-\pi(x)}$

$b(\theta(x)) = m \log(1 + e^{\theta(x)})$

$\mu(x) = b'(\theta(x)) = \frac{m}{1+e^{\theta(x)}} e^{\theta(x)} = m\,\pi(x)$ ✓

$\mathrm{var}(y) = b''(\theta(x)) = m\,\pi(x)(1-\pi(x))$

$\theta(x) = g(\mu(x))$

$= \log \frac{\frac{\mu(x)}{m}}{1 - \frac{\mu(x)}{m}}$

$= \log \frac{\mu(x)}{m - \mu(x)}$

$g(t) = \log \frac{t}{m-t}$

Examples

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Poisson regression

$$\log p(y_i \mid x_i, \beta, \sigma^2) = y_i \overbrace{\log \tilde{\mu}_i}^{\theta_i} - \overbrace{\tilde{\mu}_i}^{b(\theta)} - \overbrace{\log(y_i!)}^{c}$$

$\sigma^2 = 1$

$\theta(x) = \log \tilde{\mu}(x)$

$b(\theta(x)) = e^{\theta(x)}$

$\mu(x) = b'(\theta(x)) = e^{\theta(x)} = \tilde{\mu}(x)$ ✓

$\mathrm{var}(y) = b''(\theta(x)) = e^{\theta(x)} = \tilde{\mu}(x)$ ✓

$\theta(x) = g(\mu(x))$

$= \log \tilde{\mu}(x)$

$= \log \mu(x)$

$g(t) = \log(t)$

log link fcn

ML Estimation

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

$\theta_i = \beta^T x_i$

- Maximize the log-likelihood

$$\log p(y_1, \ldots, y_n \mid \beta) = \sum_{i=1}^{n} \frac{y_i \theta_i - b(\theta_i)}{\sigma^2} + \text{const}$$

$$\frac{d\ell_i}{d\beta_j} = \frac{d\ell_i}{d\theta_i}\frac{d\theta_i}{d\beta_j} = \sum_{i=1}^{n} \frac{y_i - b'(\theta_i)}{\sigma^2} \cancel{\frac{d\theta_i}{d\beta_j}}\, x_{ij} = 0$$

- No closed-form solution, so use iterative methods
  - 2nd order methods like IRLS require Hessian

$$H = -\frac{1}{\sigma^2} X^T S X \qquad S = \mathrm{diag}\left(\frac{d\mu_1}{d\theta_1}, \ldots, \frac{d\mu_n}{d\theta_n}\right)$$

ML Estimation

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- IRLS Newton updates: iteratively reweighted LS

$$\beta_{t+1} = (X^T S_t X)^{-1} X^T S_t z_t$$

$$z_t = \theta_t + S_t^{-1}(y - \mu_t)$$

$$\theta_t = X\beta_t \qquad \mu_t = g^{-1}(X\beta_t)$$

Nonparametrics + GLMs

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Consider a more general form

$$g(\mu(x)) = f(x) \qquad \theta(x) = g(\mu(x))$$

prev. $= \beta^T x$

- Can consider many forms for *f*(x) that we have studied in this course, e.g.
  - Smoothing splines ✓
  - Penalized regression splines ✓
  - Local regression (kernel methods) ✓
  - …

Smoothing Splines + GLMs

- For the standard L_2 loss we considered a penalized RSS:

$$\min_f \underbrace{\sum_{i=1}^{n}(y_i - f(x_i))^2}_{RSS(f)} + \lambda \int f''(x)^2 dx$$

$y = f(x) + \varepsilon$

  - With normal, additive errors, this is equivalent to penalized log-likelihood

$$\underset{f}{\cancel{\min}\ \max} \sum_{i=1}^{n} \log p(y_i \mid x_i, f) - \frac{1}{2}\lambda \int f''(x)^2 dx$$

$\hookrightarrow -\frac{1}{2} RSS$

  - For GLMs, we just use the specified exponential family distribution instead of a normal likelihood

Smoothing Splines + GLMs

- Penalized log-likelihood with a roughness penalty

$$\overset{\text{max}}{\cancel{\min_f}} \sum_{i=1}^{n} \log p(y_i \mid x_i, f) - \frac{1}{2}\lambda \int f''(x)^2 dx$$

- Example = ***logistic regression***

Bernoulli observations

$= p(y_i = 1 \mid \pi_i)$

$$\log p(y_i \mid x_i) = y_i \underbrace{\log\left(\frac{p(x_i)}{1 - p(x_i)}\right)}_{\theta(x)} + \log(1 - p(x_i))$$

modeled as

$$\log p(y_i \mid x_i, f) = y_i f(x_i) - \log(1 + e^{f(x_i)})$$

$\theta(x_i) = f(x_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right)$ logit link

Smoothing Splines + GLMs

- Penalized log-likelihood with a roughness penalty

$$\overset{\text{max}}{\cancel{\min_f}} \sum_{i=1}^{n} \frac{y_i f(x_i) - b(f(x_i))}{\sigma^2} - \frac{1}{2}\lambda \int f''(x)^2 dx$$

- Result is a finite-dimensional natural (cubic) spline with knots at the unique values of x, just as before

$$f(x) = \sum_{j=1}^{n} N_j(x)\beta_j$$

- In solns, replace X with N as the design matrix

- Must acct for λ ... more later

Penalized Reg. Splines + GLMs

- Penalized log-likelihood with a roughness penalty

$$\ell_p \quad \overset{\max}{\cancel{\min}}_f \underbrace{\sum_{i=1}^{n} \frac{y_i f(x_i) - b(f(x_i))}{\sigma^2}}_{\ell} - \frac{\lambda}{2}\beta^T D \beta$$

$f(x_i) = \theta_i$

some form for penalizing bases

- Recall that *f* is assumed to be some spline basis expansion
- Derivative with respect to β_j

$$\frac{\partial \ell}{\partial \beta_j} = \frac{\partial \ell}{\partial \theta_i}\frac{\partial \theta_i}{\partial \beta_j} = \sum_{i=1}^{n} \frac{y_i - b'(\theta_i)}{\sigma^2} \frac{\partial \theta_i}{\partial \beta_j}, \quad \frac{\partial \theta_i}{\partial \beta_j} = \frac{1}{\frac{\partial \mu_i}{\partial \theta_i}} \frac{d\mu_i}{d\beta_j}, \quad \mu_i = b'(\theta)$$

$$= \sum_{i=1}^{n} \frac{y_i - b'(\theta_i)}{\sigma^2} \frac{1}{b''(\theta_i)} \frac{d\mu_i}{d\beta_j}$$

overall

$$\frac{\partial \ell_p}{\partial \beta_j} = \sum_{i=1}^{n} \frac{y_i - \mu_i}{\sigma^2} \frac{1}{V_i} \frac{d\mu_i}{d\beta_j} - \lambda D \beta_j = 0$$

Penalized Reg. Splines + GLMs

- Penalized log-likelihood with a roughness penalty

$$\frac{d\ell_p}{d\beta_j} = \sum_{i=1}^{n} \frac{d\mu_i}{d\beta_j}\frac{y_i - \mu_i}{\sigma^2 V_i} - \lambda D \beta_j = 0$$

- Again, no closed-form solution as with parametric GLMs
- Use “penalized” IRLS

$$\beta_{t+1} = (X^T S_t X + \underline{\lambda D})^{-1} X^T S_t z_t$$
$$z_t = \theta_t + S_t^{-1}(y - \mu_t)$$
$$S_t = \mathrm{diag}\left(\frac{d\mu_1/d\theta_1}{\sigma^2 V_1}, \ldots, \frac{d\mu_n/d\theta_n}{\sigma^2 V_n}\right)$$

- Return: $L^\lambda = X(X^T S X + \underline{\lambda D})^{-1} X^T S$ hat matrix

Local Linear Regression

- Consider locally weighted linear regression instead
- Local linear model around fixed target x_0 :

$$\beta_{0x_0} + \beta_{1x_0}(x - x_0)$$ ← center fit around target location

- Minimize:

kernel

$$\min_{\beta_{x_0}} \sum_i K_\lambda(x_0, x_i)\left(\underbrace{y_i - \beta_{0x_0} - \beta_{1x_0}(x_i - x_0)}_{\text{RSS}}\right)^2$$

weight close obs. more

- Return: $\hat{f}(x_0) = \hat{\beta}_{0x_0}$ ← fit at x_0

Note: not equivalent to fitting a local constant!

- Fit a new local polynomial for *every* target x_0

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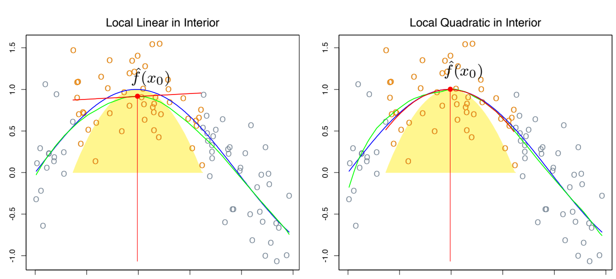
Local Polynomial Regression

- Local linear regression is biased in regions of curvature
  - "Trimming the hills" and "filling the valleys"
- Local quadratics tend to eliminate this bias, but at the cost of increased variance



From Hastie, Tibshirani, Friedman book

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Local Polynomial Regression

- ~~Consider local polynomial of degree *d* centered about x_0~~

$$\boxed{P_{x_0}(x;\beta_{x_0}) = \beta_{0x_0} + \beta_{1x_0}(x-x_0) + \frac{\beta_{2x_0}}{2!}(x-x_0)^2 + \cdots + \frac{\beta_{dx_0}}{d!}(x-x_0)^d}$$

- Minimize: $\min_{\beta_{x_0}} \sum_{i=1}^{n} K_\lambda(x_0,x_i)(y_i - P_{x_0}(x;\beta_{x_0}))^2$
- Equivalently:

$$\min_{\beta_{x_0}} (y - X_{x_0}\beta_{x_0})^T W_{x_0} (y - X_{x_0}\beta)$$

$$X_{x_0} = \begin{bmatrix} 1 & x_1 - x_0 & \cdots & \frac{(x_1-x_0)^d}{d!} \\ \vdots & & & \\ 1 & x_n - x_0 & \cdots & \frac{(x_n-x_0)^d}{d!} \end{bmatrix}$$

- Return: $\hat{f}(x_0) = \hat{\beta}_{0x_0}$
- Bias only has components of degree *d+1* and higher

Local Likelihood Methods

- Just as with spline methods, replace RSS with log-likelihood
- For $\theta_i = x_i^T\beta$

$$\ell(\beta) = \sum_{i=1}^{n} \ell(y_i, x_i^T\beta)$$

parametric GLM

- Under a local polynomial model,

$$\ell(\beta) = \sum_{i=1}^{n} K_\lambda(x_0,x_i)\ell(y_i, P_{x_0}(x_i;\beta))$$

polynomial around x_0, as before

consider sum of log-like terms, but weighted by proximity to x_0 (locally)

Local Likelihood Methods

$$\ell(\beta) = \sum_{i=1}^{n} K_\lambda(x_0, x_i)\ell(y_i, P_{x_0}(x_i; \beta))$$

- Example: ***multiclass logistic regression***
- For

$$Pr(G = j \mid X = x) = \frac{e^{\beta_{j0} + \beta_j^T x}}{1 + \sum_{k=1}^{J-1} e^{\beta_{k0} + \beta_k^T x}}$$

- Under a local polynomial model,

$$\sum_{i=1}^{n} \underbrace{K_\lambda(x_0, x_i)}_{\text{weights}} \Bigg\{ \beta_{g_i 0}(x_0) + \beta_{g_i}(x_0)^T (x_i - x_0)$$

obs i ... pick out correct term

log-lik

$$- \log \left[1 + \sum_{k=1}^{J-1} \exp(\underbrace{\beta_{k0}(x_0) + \beta_k(x_0)^T (x_i - x_0)}_{\text{local polynomial = linear}}) \right] \Bigg\}$$

Local Likelihood Methods

$$\ell(\beta) = \sum_{i=1}^{n} K_\lambda(x_0, x_i)\ell(y_i, P_{x_0}(x_i; \beta))$$

- Example: ***multiclass logistic regression***
- For

$$Pr(G = j \mid X = x) = \frac{e^{\beta_{j0} + \beta_j^T x}}{1 + \sum_{k=1}^{J-1} e^{\beta_{k0} + \beta_k^T x}}$$

- Return:

$$\hat{P}_r(G = j \mid X = x_0) = \frac{e^{\hat{\beta}_{j0}(x_0)}}{1 + \sum_{k=1}^{J-1} e^{\hat{\beta}_{k0}(x_0)}}$$

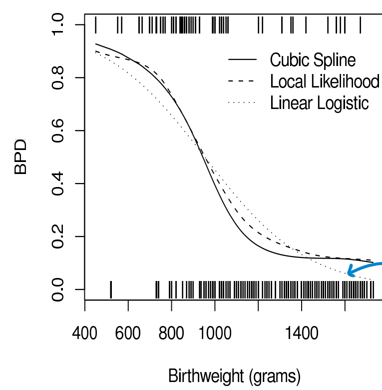
target location

Example

- Bronchopulmonary dysplasia (BPD) and birthweight data
- Logistic regression model with binomial observations

$$\log p(y_i \mid x_i, f) = y_i f^{\lambda}(x_i) - n_i \log(1 + e^{f^{\lambda}(x_i)})$$

- Choose λ by AIC
- Notice that behavior for high birthweights is quite different from that of linear logistic model



From Wakefield textbook

linear logistic
$\theta_i = \beta^T x_i$

Example

- Bronchopulmonary dysplasia (BPD) and birthweight data
- Logistic regression model with binomial observations

$$\log p(y_i \mid x_i, f) = y_i f^{\lambda}(x_i) - n_i \log(1 + e^{f^{\lambda}(x_i)})$$

- For the local likelihood fit, we have

$$\ell(\beta) = \sum_{i=1}^{n} K_{\lambda}(x_0, x_i) n_i \left[\frac{y_i}{n_i} P_{x_0}(x_i; \beta) - \log(1 + e^{P_{x_0}(x_i;\beta)}) \right]$$

polynomial

- Fit uses tri-cube kernel

Local Fits of Autoregressions

$$\ell(\beta) = \sum_{i=1}^{n} K_\lambda(x_0, x_i)\ell(y_i, P_{x_0}(x_i;\beta))$$

- An autoregressive time series model of order *k*

$$\begin{aligned} y_t &= \beta_0 + \beta_1 y_{t-1} + \beta_2 y_{t-2} + \cdots + \beta_k y_{t-k} + \epsilon_t \\ &= z_t^T \beta + \epsilon_t \end{aligned}$$

$z_t = [1\ y_{t-1}, \ldots, y_{t-k}]$

- Using a local likelihood approach, can consider kernel

$$K_\lambda(z_0, z_t)$$

- Allows for fit of the autoregressive coefficients to vary in time by considering only a short history