Representing Additive Models as Mixed Models

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LMU Seminar: Mixed and Semiparametric Models

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Truncated Power Basis

univariate:

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + ... + \theta_d x^d + \sum_{k=1}^{K} \theta_{dk} (x - \kappa_k)_+^d + \epsilon$$

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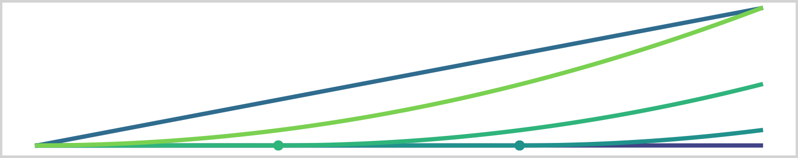
univariate and quadratic with two knots:

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_{21}(x - \kappa_1)_+^2 + \theta_{22}(x - \kappa_2)_+^2 + \epsilon$$



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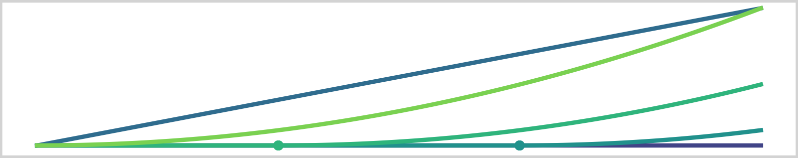
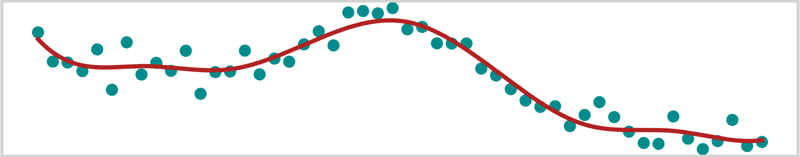


Additive Models

Semiparametric regression:

$$\hat{y}_i = f(\nu_i) + u_i^T \gamma$$



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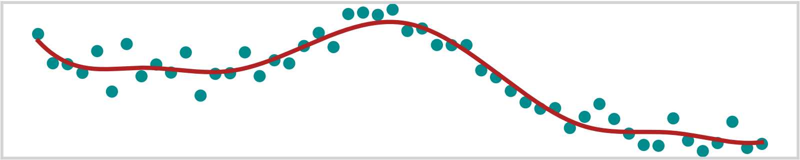

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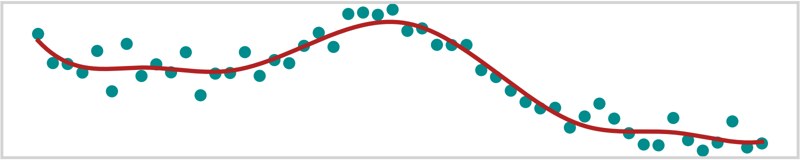
In matrix notation:

$$\hat{y} = V\xi + U\gamma$$



Additive Models

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$$\hat{y}_i = \overbrace{f_1(\nu_{i1})}^{v_{i1}^T \xi_1} + \ldots + \overbrace{f_p(\nu_{ip})}^{v_{ip}^T \xi_p} + u_i^T \gamma$$

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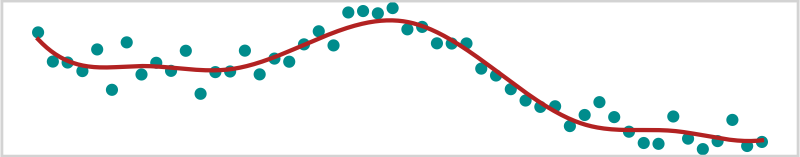

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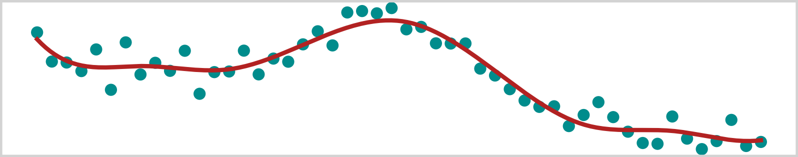
In matrix notation:

$$\hat{y} = V_1 \xi_1 + \ldots + V_p \xi_p + U\gamma = \sum_{j=1}^{p} V_j \xi_j + U\gamma$$



Splines

Spline functions are **piecewise polynomial segments** (called basis functions) joined together smoothly at so-called knots.

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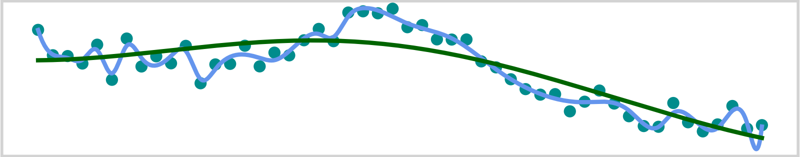
with basis functions $b_1(.), ..., b_k(.)$, e. g. *B-spline*, truncated power basis, natural cubic spline, ...

Roughness Penalty

Penalized Regression Spline:

$$\log L(\xi, \gamma) + \lambda \int_{x_1}^{x_n} \left[f''(x) \right]^2 dx$$

Control wiggliness (bias-variance tradeoff):

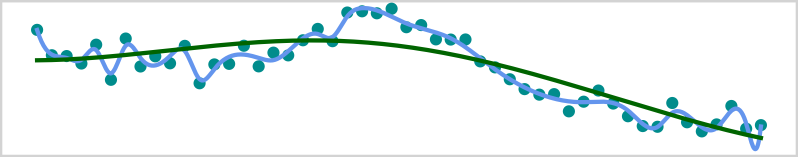


Roughness Penalty

Penalized Regression Spline:

$$\log L(\xi, \gamma) + \lambda \xi^T K \xi$$

e. g. first order differences $\xi^T K \xi = \sum(\xi_{k+1} - \xi_k)^2$:



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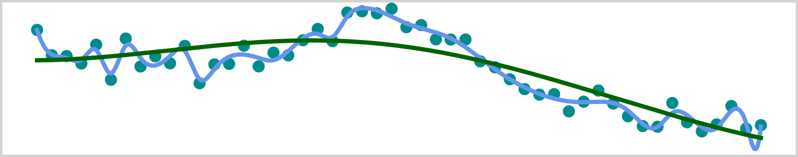
Problem: How to choose λ?



Mixed Models

$$y_i = \underbrace{X_i \beta}_{\text{fixed effects}} + \overbrace{Z_i b_i}^{\text{random effects}} + \epsilon_i$$

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Empirical Bayes

- **Idea:** Use Mixed Model inference: $y = \sum_{j=1}^{p} \underbrace{V_p \xi_p}_{\text{random effects}} + \overbrace{U\gamma}^{\text{fixed effects}} + \epsilon$

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$$\max_{\tau_1, ..., \tau_p} \log L(\gamma, \xi_1, ..., \xi_p) - \sum_{j=1}^{p} \underbrace{\frac{1}{2\tau_j^2}}_{\lambda_j} \xi_j^T \underbrace{\Sigma_j^{-1}}_{K_j} \xi_j$$

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$\Rightarrow$ Empirical Bayes is equivalent to penalized Maximum Likelihood

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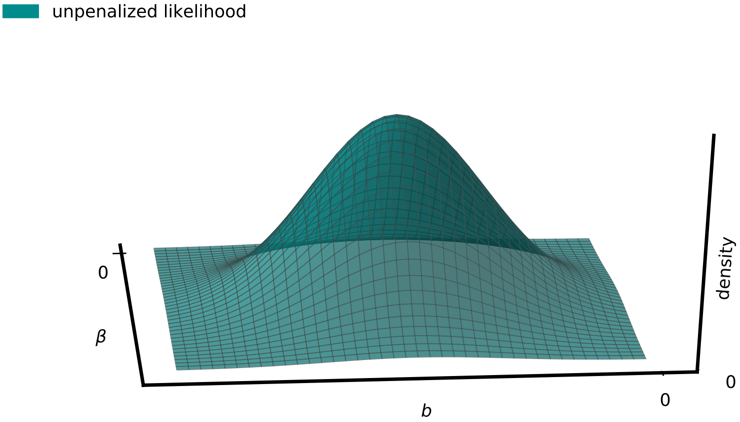
- b: penalized parts with a proper (Gaussian) prior
  $\dim(b_j) = \text{rank}(K_j)$

Mixed Model Representation



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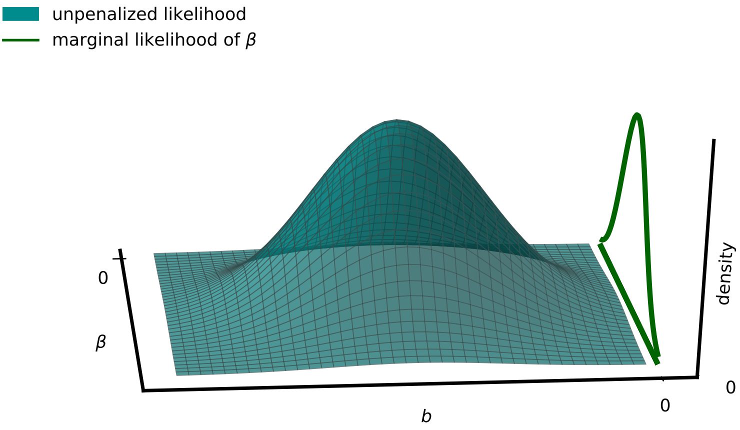

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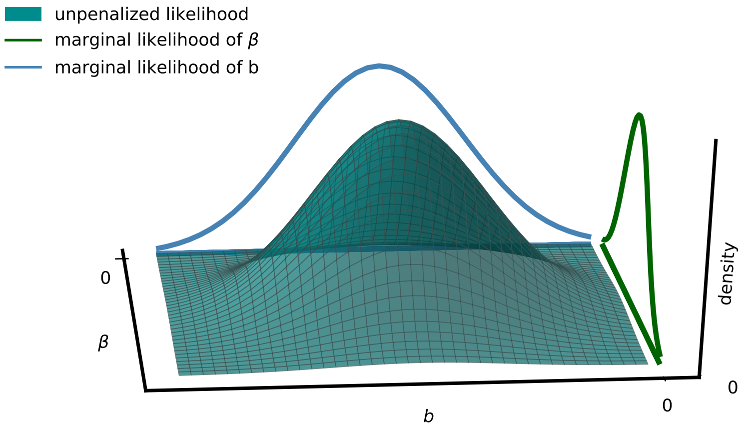

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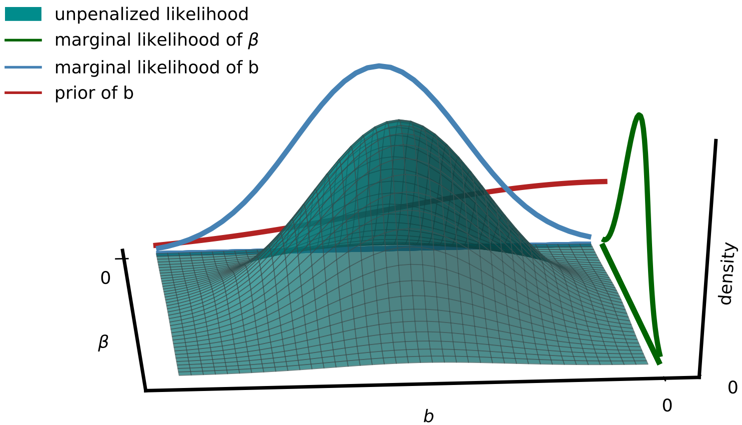

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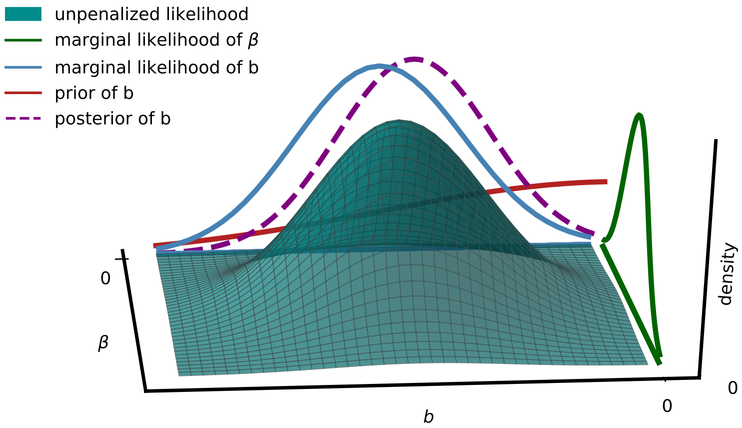

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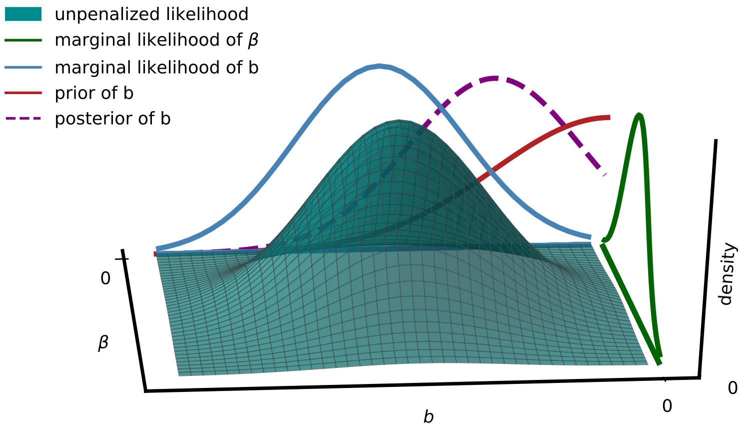

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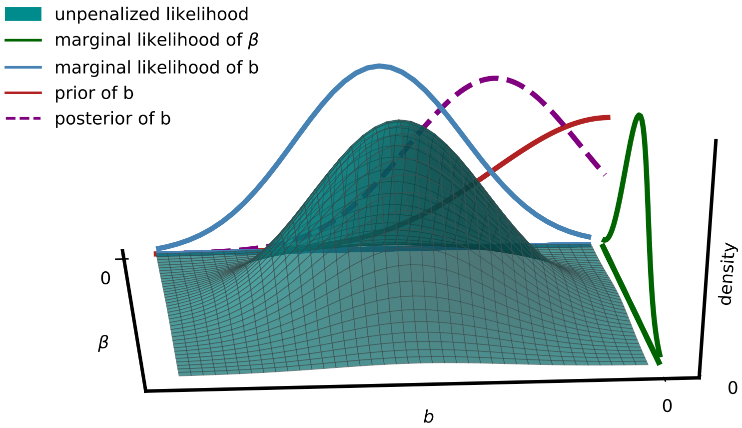

The lower the prior variance, the higher the penalty!

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$$\beta := (\beta_1^T, ..., \beta_p^T, \gamma^T)$$

$$b := (b_1^T, ..., b_p^T)$$

$$Z := V_j\tilde{Z}_j$$

$$X := (V_j\tilde{X}_j, U)$$

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3. β_j not penalized by K_j: $\tilde{X}_j^T K_j \tilde{X}_j = 0$
4. Gaussian prior for b_j: $\tilde{Z}_j^T K_j \tilde{Z}_j = I_{kj}$

Choosing $\tilde{X}_j$ and $\tilde{Z}_j$ for Mixed Model Representation

Recap: Requirements

1. 1-on-1 transformation: matrix $(\tilde{X}_j \;\; \tilde{Z}_j)$ has full rank
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Setup

- $\tilde{X}_j$ is a basis of the null space of K_j (condition 3)
- $\tilde{Z}_j = L_j(L_j^T L_j)^{-1}$ with $K_j = L_j L_j^T$ (conditions 1 and 4)
- Choose L_j s. t. $L_j^T \tilde{X}_j = 0$ and $\tilde{X}_j L_j^T = 0$ (condition 2)
  e. g. spectral decomposition: $K_j = \Gamma_j \Lambda_j \Gamma^T$, so $L_j = \Gamma \Lambda_j^{1/2}$

Mixed Model Representation

log-Prior:

$$\log p(\xi_j|\tau_j^2) \propto -\frac{1}{2\tau_j^2}\xi_j^T K_j \xi_j$$

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$\Rightarrow p(\beta) \propto$ const.

Mixed Model Representation

log-Prior:

$$\log p(\xi_j|\tau_j^2) \propto -\frac{1}{2\tau_j^2}\xi_j^T K_j \xi_j = -\frac{1}{2\tau_j^2} b_j^T b_j$$

$\Rightarrow p(\beta) \propto$ const.
$\Rightarrow p(b_j) \sim N(0, \tau_j^2 I_{kj})$

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log-Posterior:

$$l_p(\beta, b|y) = l(y, \beta, b) - \sum_{j=1}^{p} \overbrace{\frac{1}{2\tau_j^2}}^{=\lambda} b_j^T b_j$$

Estimates $\hat{\beta}$ and $\hat{b}$

In order to maximize the (log-)Posterior (equivalent to ML), derive estimates for β and b simultaneously based on known σ^2 and τ^2.

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Mixed Model equations:

$$\overbrace{\begin{pmatrix} X^T WX & X^T WZ \\ Z^T WX & Z^T WZ + Q^{-1} \end{pmatrix}}^{\text{Fisher information}} \begin{pmatrix} \hat{\beta} \\ \hat{b} \end{pmatrix} = \begin{pmatrix} X^T Wy \\ Z^T Wy \end{pmatrix}$$

with $W = \text{diag}(\sigma^2)$ and $Q = \text{blockdiag}(\tau_1^2 I_{k1}, ..., \tau_p^2 I_{kp})$

Variance Estimates

Maximum Likelihood (integrate b out)

- uses (partially) marginal distribution $y \sim \mathrm{N}(X\beta, \Sigma)$
  1. Derive $\hat{\beta}$ analytically
  2. Plug in to get profile likelihood for τ^2 and σ^2
  3. Maximize numerically
- estimates variance components of posterior mode

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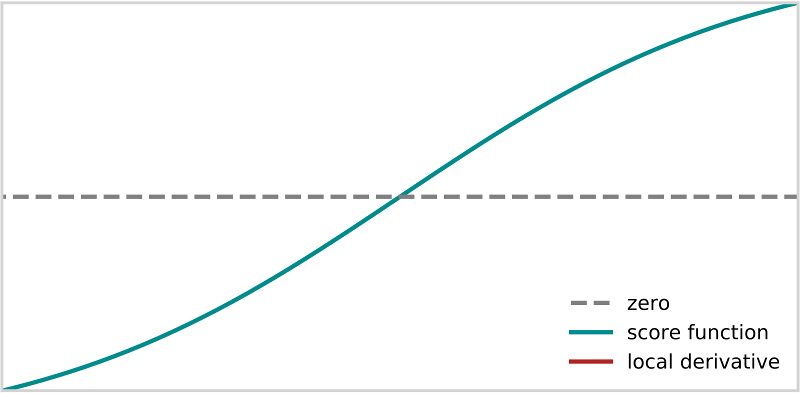
Restricted ML (integrate b and β out)

- directly uses marginal distribution of y
- Advantages over ML:
  + considers loss of degrees of freedom due to estimation of β
  + estimates mode of the marginal posterior for the variances

Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

Maximize the restricted likelihood (REML) using Newton-Raphson:



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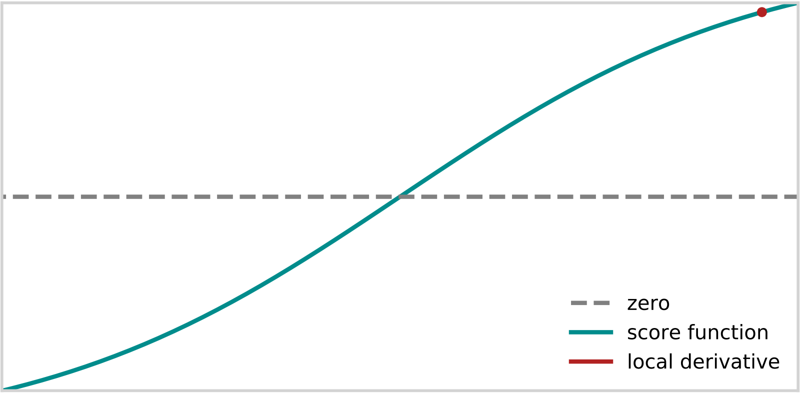

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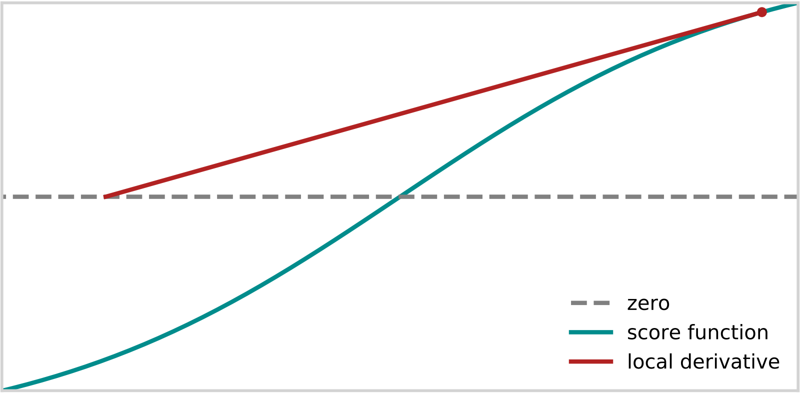

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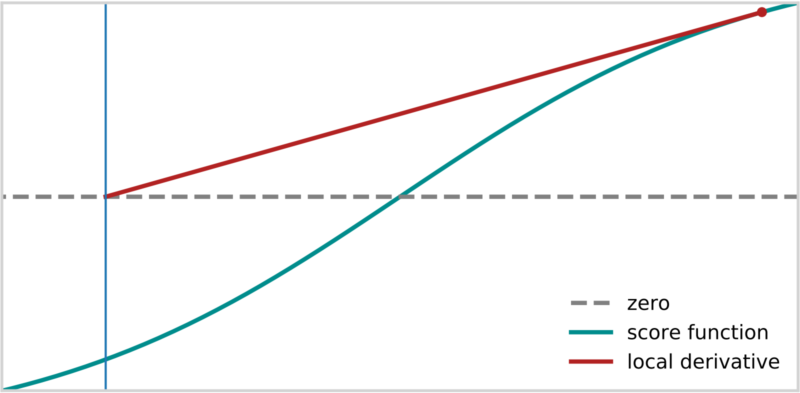

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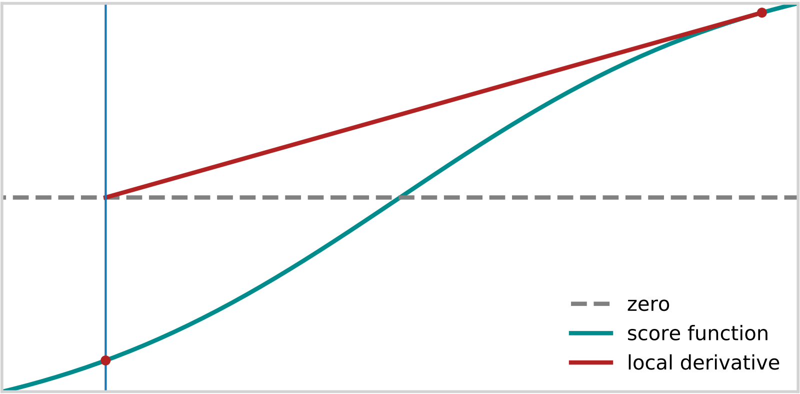

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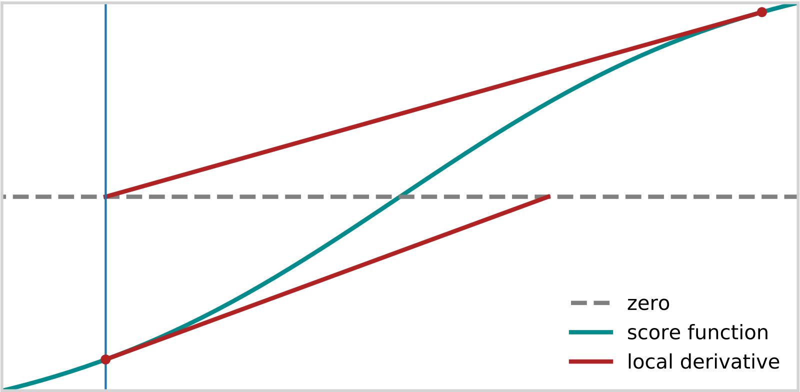

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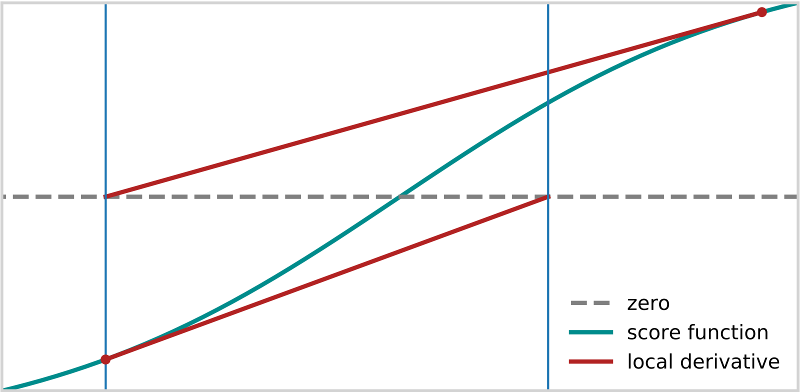

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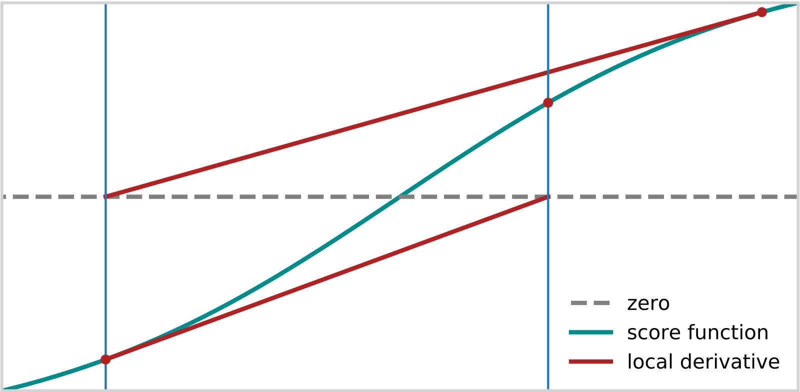

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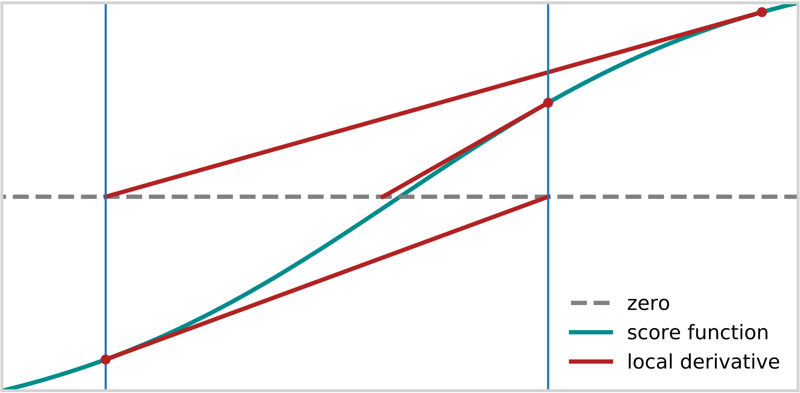

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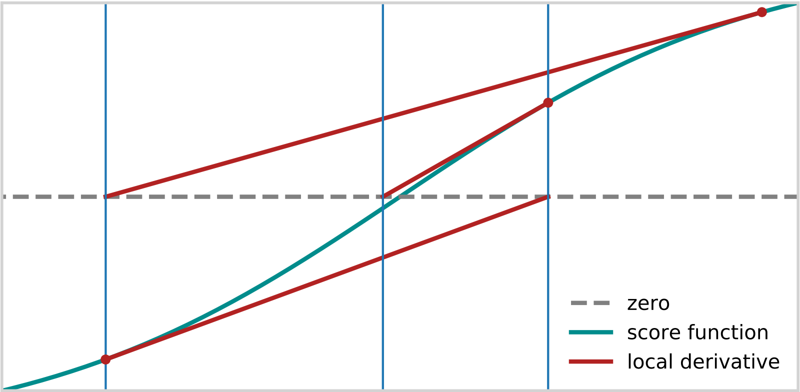

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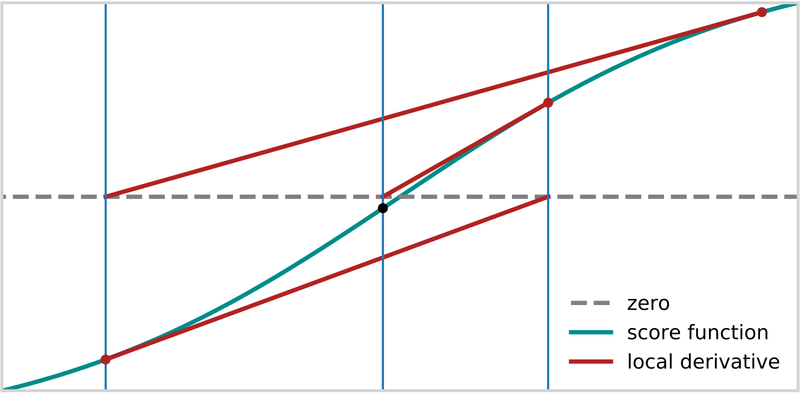

(RE)ML estimation

Single iterations (old)

- **Update $\hat{\beta}$ and $\hat{\boldsymbol{b}}$** given the current $\hat{\lambda}$
- **Update $\hat{\boldsymbol{\lambda}}$** using Fisher-Scoring (or Newton-Raphson)
  $\rightarrow \mathcal{V}_{\hat{\beta},\hat{\boldsymbol{b}}}(\lambda)$ depends on $\hat{\beta}$ and $\hat{\boldsymbol{b}}$

$\Rightarrow$ Convergence is not guaranteed

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Nested iterations (new)

- **Update $\hat{\boldsymbol{\lambda}}$** using Newton-Raphson
  - **Estimate $\hat{\boldsymbol{\beta}}_{\boldsymbol{\lambda}}$ in an inner loop**

  $\rightarrow \mathcal{V}(\lambda)$ depends on β and b only via $\hat{\beta}_\lambda$ and $\hat{b}_\lambda$
- **Update $\hat{\boldsymbol{\beta}}$ and $\hat{\boldsymbol{b}}$** given the current $\hat{\lambda}$

$\Rightarrow$ Convergence is guaranteed (under mild regulatory conditions)

Comparison of Mixed Model Approach

Fully Bayesian approach (MCMC)

+ no reparameterization needed
– how to choose hyperpriors?
– Markov chain convergence is difficult to determine

Prediction error methods (AIC, GCV)

+ better prediction error performance
– worse resistance to overfit
– higher smoothing parameter variability
– increased tendency to multiple minima

$\rightarrow$ *more on that next week*

Summary

- Semiparametric models can be **written as mixed models**.
- In order to get a proper random effects distribution, the flexible parameters have to be **separated** into sets of parameters with **flat priors** and sets with **proper priors**.
- The penalty term is proportional to the inverse of the prior variance: $\boldsymbol{\lambda} \propto \frac{1}{\boldsymbol{\tau}^2}$
- For good results in mixed model inference, the **penalty term** has to be estimated in a **nested iteration** setup with the other parameters.

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