

Representing Additive Models as Mixed Models

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LMU Seminar: Mixed and Semiparametric Models

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Truncated Power Basis

univariate:

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

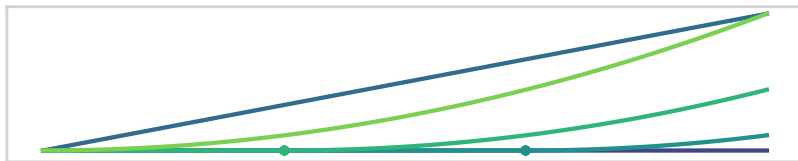
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univariate and quadratic with two knots:

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



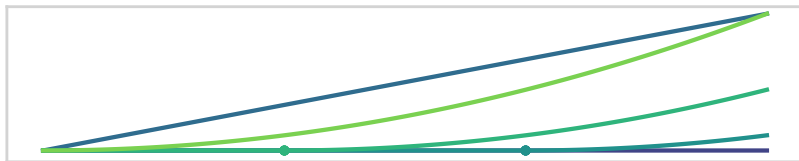
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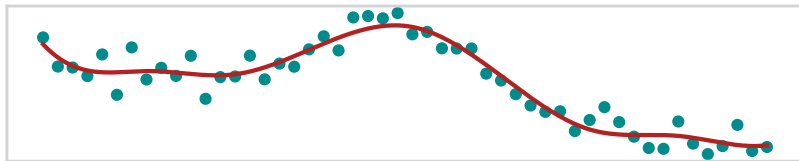
$$y = \overbrace{\theta_0 + \theta_1 x + \theta_2 x^2}^{\text{fixed effects}} + \overbrace{\theta_{21}(x - \kappa_1)_+^2 + \theta_{22}(x - \kappa_2)_+^2}^{\text{random effects: depend on } i} + \epsilon$$



Additive Models

Semiparametric regression:

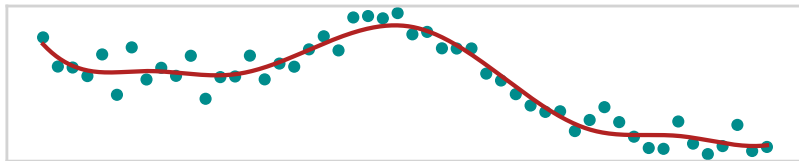
$$\hat{y}_i = f(\nu_i) + u_i^T \gamma$$



Additive Models

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



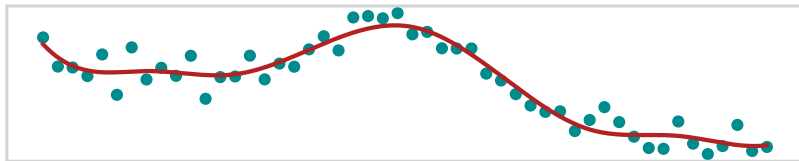
Additive Models

Semiparametric regression:

$$\hat{y}_i = \underbrace{v_i^T \xi}_{f(v_i)} + u_i^T \gamma$$

In matrix notation:

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

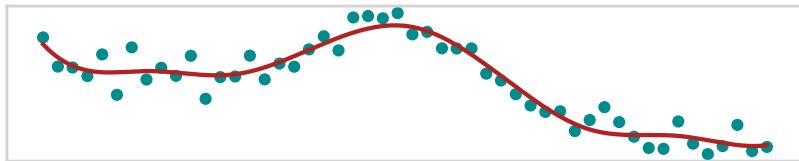


Additive Models

Semiparametric regression:

$$\hat{y}_i = \underbrace{f_1(\nu_{i1})}_{\nu_{i1}^T \xi_1} + \dots + \underbrace{f_p(\nu_{ip})}_{\nu_{ip}^T \xi_p} + u_i^T \gamma$$

In matrix notation:



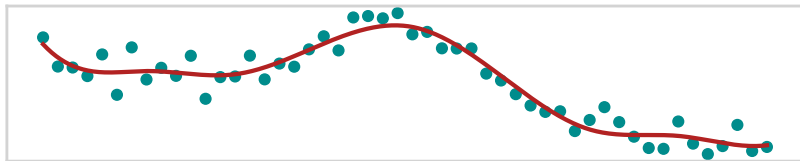
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In matrix notation:

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



Splines

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

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$$\hat{y} = V\xi + U\gamma = \begin{pmatrix} b_1(x_1) & \dots & b_k(x_1) \\ \vdots & \ddots & \vdots \\ b_1(x_n) & \dots & b_k(x_n) \end{pmatrix} \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_k \end{pmatrix} + \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix}$$



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

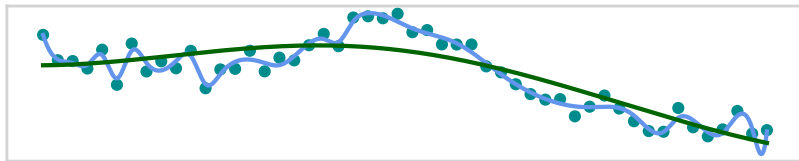


Roughness Penalty

Penalized Regression Spline:

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

Control wiggleness (bias-variance tradeoff):

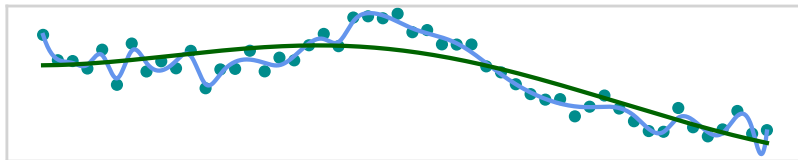


Roughness Penalty

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

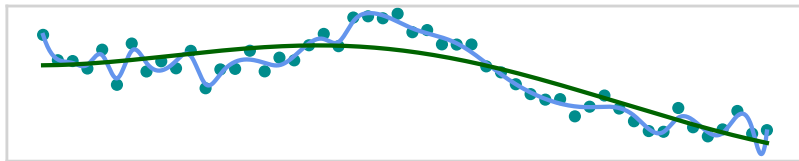


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Problem: How to choose λ ?



Mixed Models

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

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random effects induce a general linear model with **correlated errors**

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the random effects distribution is a **prior** on the random effects

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

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

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⇒ Empirical Bayes is equivalent to penalized Maximum Likelihood

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The Gaussian prior $p(\xi_j | \tau_j^2) \propto \exp\left(-\frac{1}{2\tau_j^2} \xi_j^T K_j \xi_j\right)$ is improper.

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 $\dim(\beta_j) = \dim(\xi_j) - \text{rank}(K_j)$

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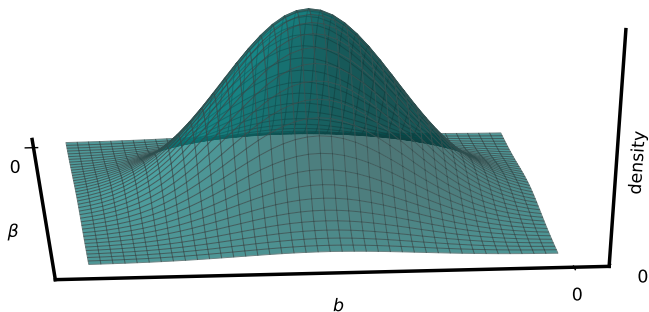
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- b : penalized parts with a proper (Gaussian) prior
 $\dim(b_j) = \text{rank}(K_j)$

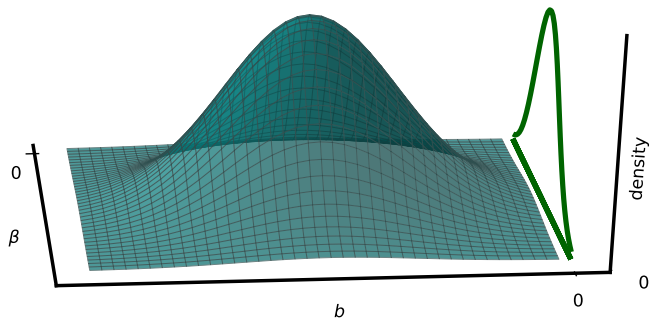
Mixed Model Representation

unpenalized likelihood



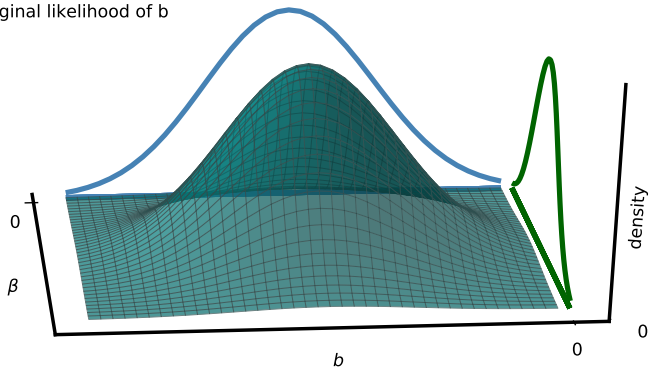
Mixed Model Representation

- unpenalized likelihood
- marginal likelihood of β



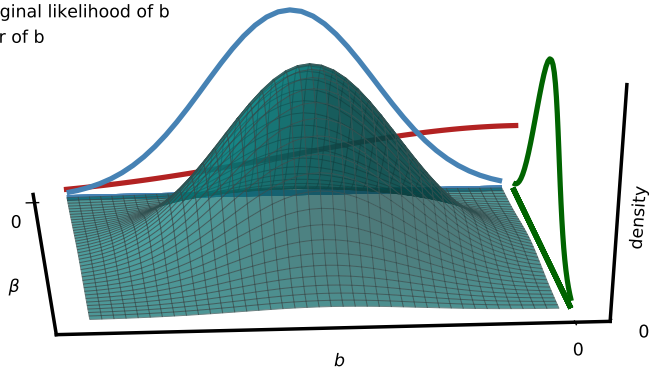
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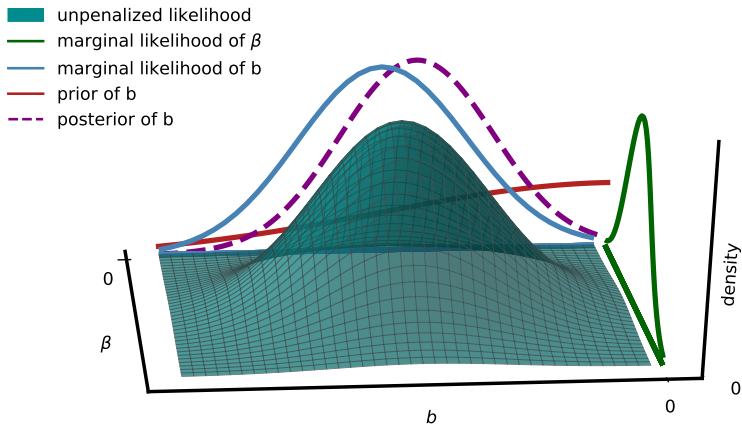


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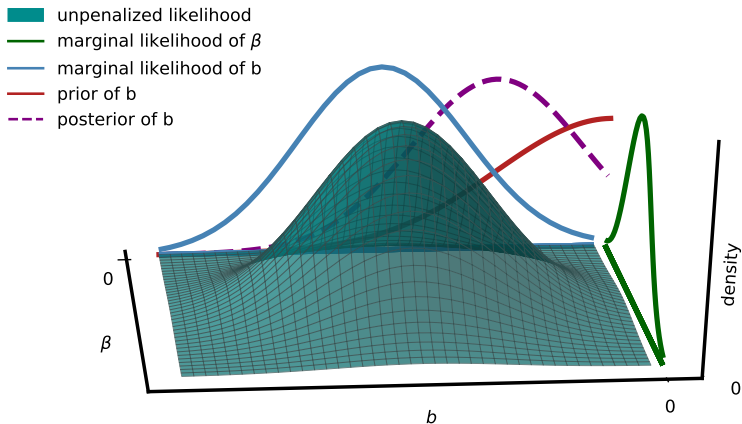
- unpenalized likelihood
- marginal likelihood of β
- marginal likelihood of b
- prior of b



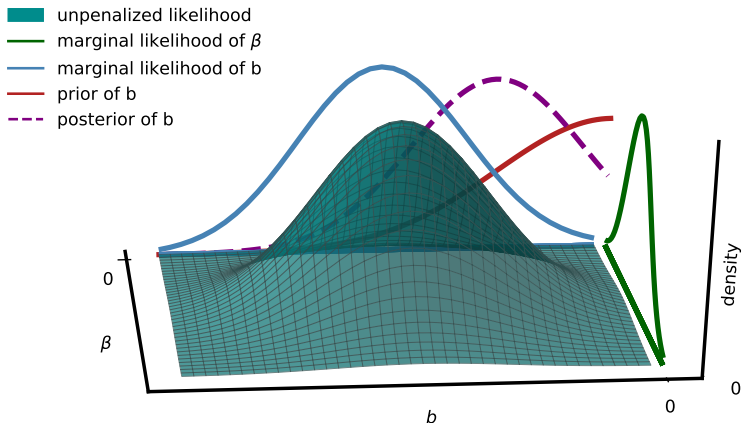
Mixed Model Representation



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The lower the prior variance, the higher the penalty!

Mixed Model Representation

Decomposition $\xi_j = \tilde{X}_j\beta_j + \tilde{Z}_jb_j$:

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$$y = \sum_{j=1}^p V_j \overbrace{(\tilde{X}_j\beta_j + \tilde{Z}_jb_j)}^{\xi_j} + U\gamma = X\beta + Zb$$

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

$$b := (b_1^T, \dots, b_p^T)$$

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

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

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4. Gaussian prior for b_j : $\tilde{Z}_j^T K_j \tilde{Z}_j = I_{k_j}$

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
2. \tilde{X}_j and \tilde{Z}_j are orthogonal: $\tilde{X}_j^T \tilde{Z}_j = 0$
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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: $K_j = \Gamma_j \Lambda_j \Gamma_j^T$, so $L_j = \Gamma \Lambda_j^{1/2}$

Mixed Model Representation

log-Prior:

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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:

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

with $W = \text{diag}(\sigma^2)$ and $Q = \text{blockdiag}(\tau_1^2 I_{k_1}, \dots, \tau_p^2 I_{k_p})$

Variance Estimates

Maximum Likelihood (integrate b out)

- uses (partially) marginal distribution $y \sim N(X\beta, \Sigma)$
 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

Variance Estimates

Maximum Likelihood (integrate b out)

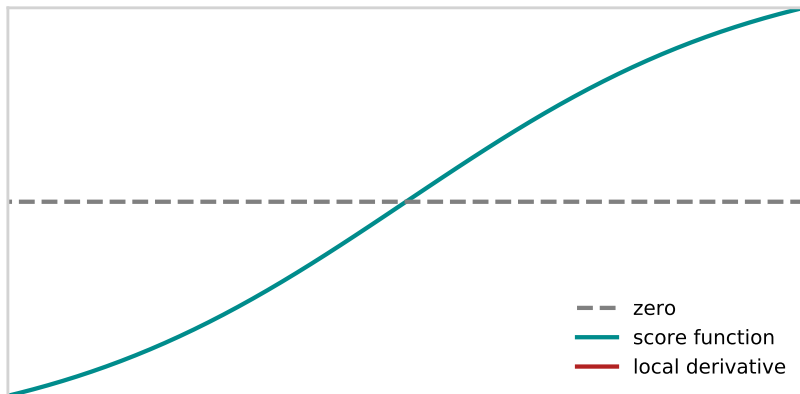
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Restricted ML (integrate b and β out)

- 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

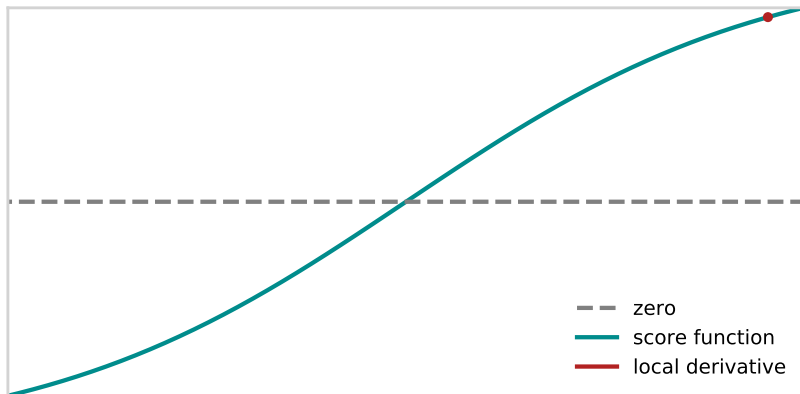
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



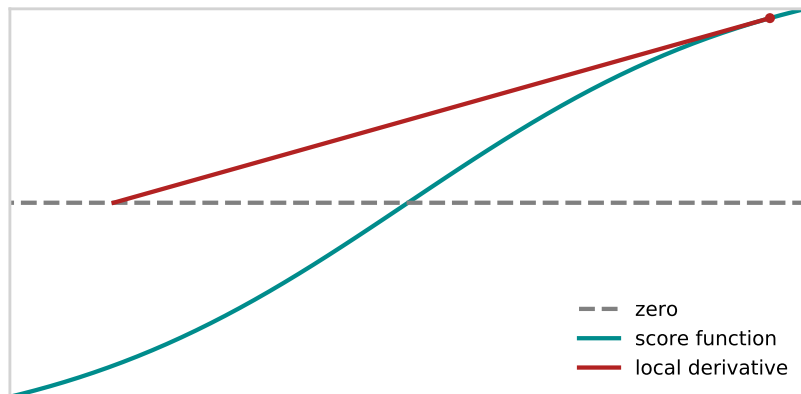
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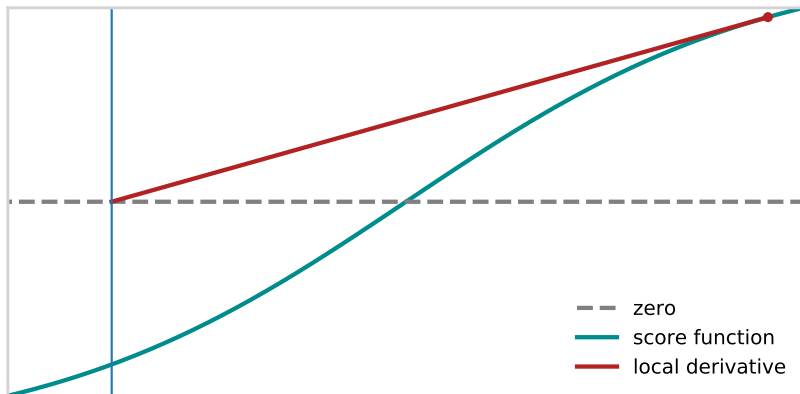
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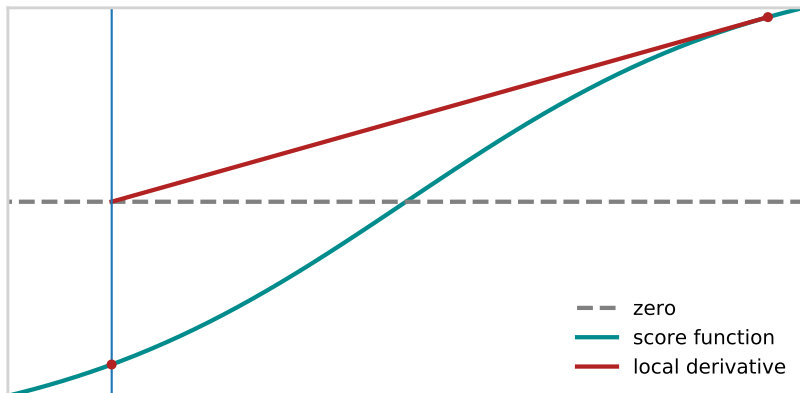
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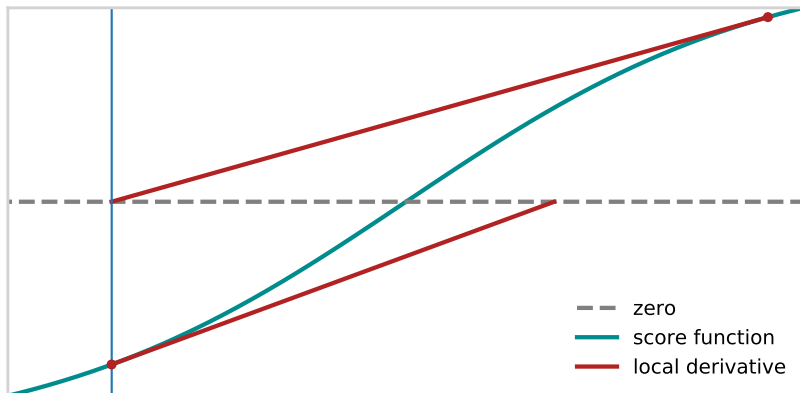
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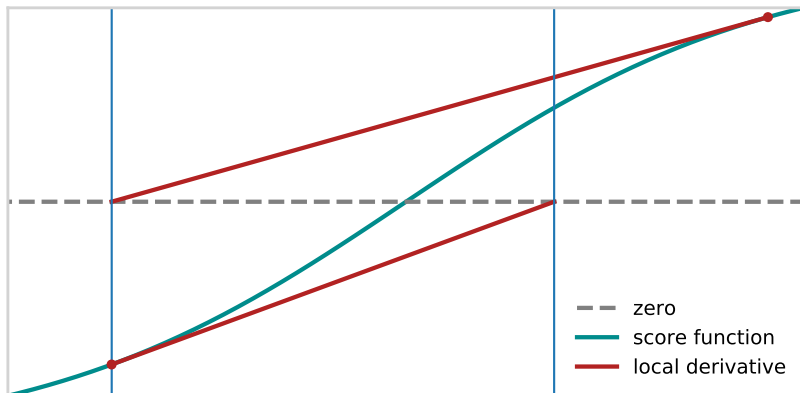
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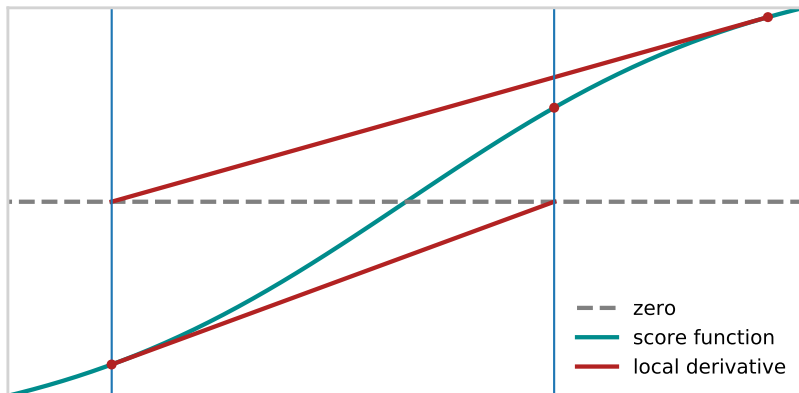
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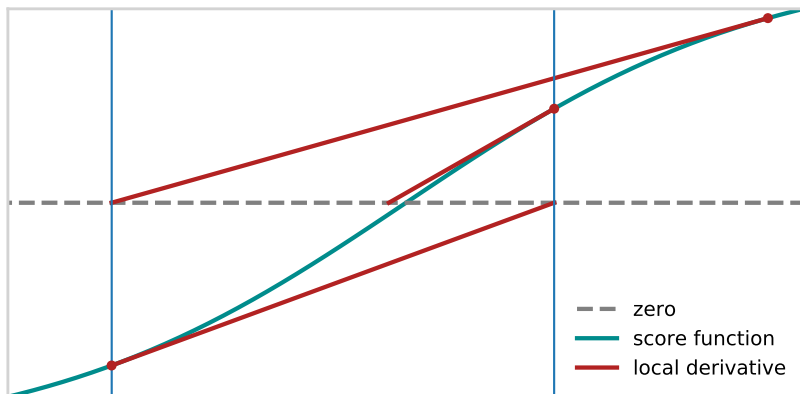
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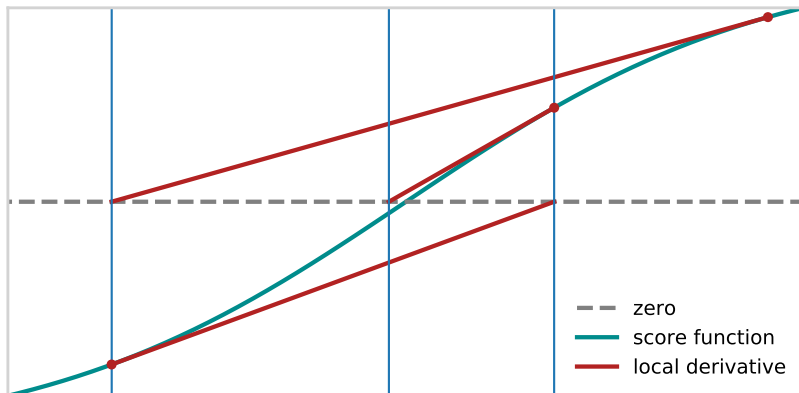
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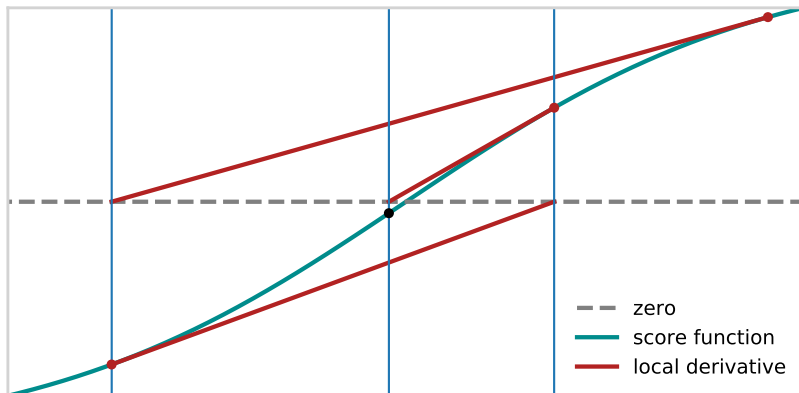
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Maximize the restricted likelihood (REML) using Newton-Raphson:



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

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



(RE)ML estimation

Single iterations (old)

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

⇒ Convergence is not guaranteed

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Nested iterations (new)

- **Update $\hat{\lambda}$** using Newton-Raphson
 - **for each step: estimate $\hat{\beta}_{\lambda}$ and \hat{b}_{λ}**
→ $\mathcal{V}(\lambda)$ depends on β and b only via $\hat{\beta}_{\lambda}$ and \hat{b}_{λ}

- **Update $\hat{\beta}$ and \hat{b}** given the current $\hat{\lambda}$

⇒ Convergence is guaranteed (under mild regulatory conditions)

Comparison of Mixed Model Approach

Fully Bayesian approach (MCMC)

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





Prediction error methods (AIC, GCV)

- + better prediction error performance
- worse resistance to overfit
- higher smoothing parameter variability
- increased tendency to multiple minima
- *more on that next week*

Summary

- Semiparametric models can be **written as mixed models**, which enables an efficient way to estimate the penalty term λ .
- 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: $\lambda \propto \frac{1}{\tau^2}$
- 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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