

Representing Additive Models as Mixed Models

Katharina Ring

LMU Seminar: Mixed and Semiparametric Models

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Truncated Power Basis

univariate:

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

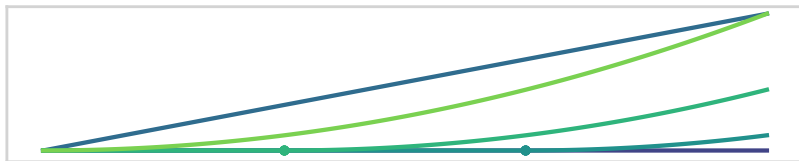
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univariate and quadratic with two knots:

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



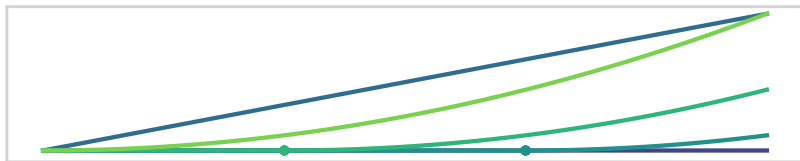
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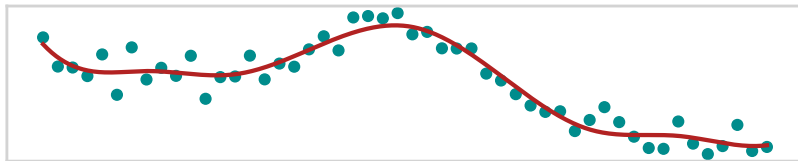
$$y = \overbrace{\theta_0 + \theta_1 x + \theta_2 x^2}^{\text{fixed effects}} + \overbrace{\theta_{21}(x - \kappa_1)_+^2 + \theta_{22}(x - \kappa_2)_+^2}^{\text{random effects: depend on } i}$$



Additive Models

Semiparametric regression:

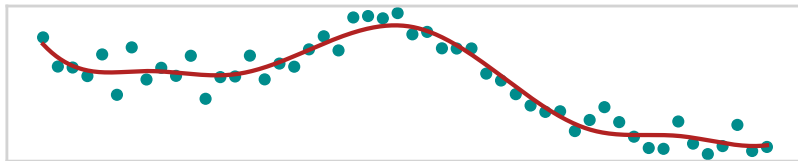
$$y_i = f(\nu_i) + u_i^T \gamma$$



Additive Models

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



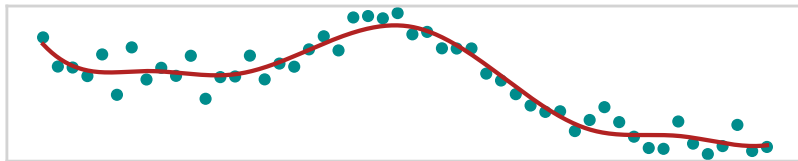
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In matrix notation:

$$y = V\xi + U\gamma$$

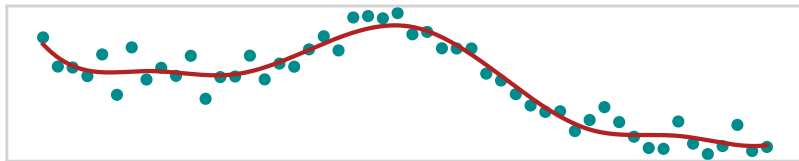


Additive Models

Semiparametric regression:

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

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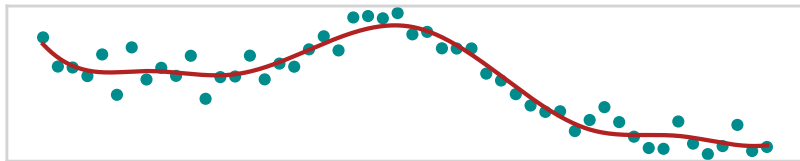
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In matrix notation:

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



Splines

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

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

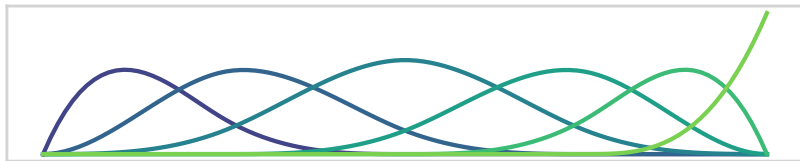


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with basis functions $b_1(\cdot), \dots, b_k(\cdot)$, e. g. *B-spline*, truncated power basis, natural cubic spline, ...

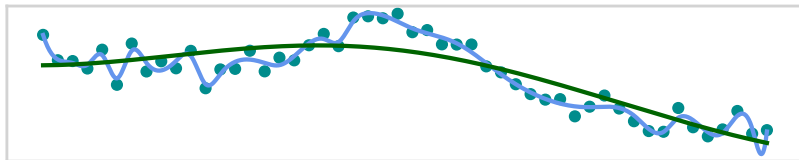


Roughness Penalty

Penalized Regression Spline:

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

Control wiggleness:

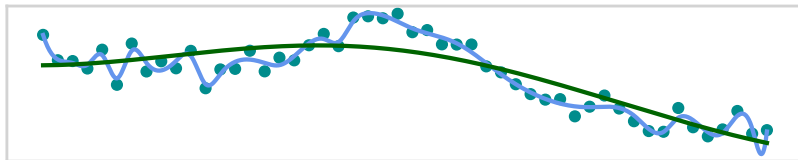


Roughness Penalty

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

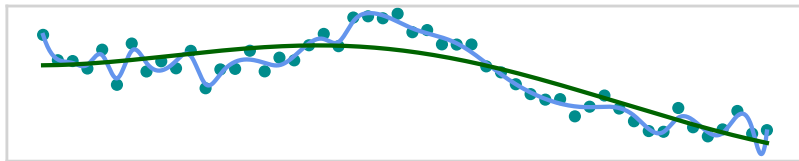


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Problem: How to choose λ ?



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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Posterior: $p(\xi_1, \dots, \xi_p, \gamma | y) \propto L(y, \xi_1, \dots, \xi_p, \gamma) \prod_{j=1}^p p(\xi_j | \tau_j^2)$

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

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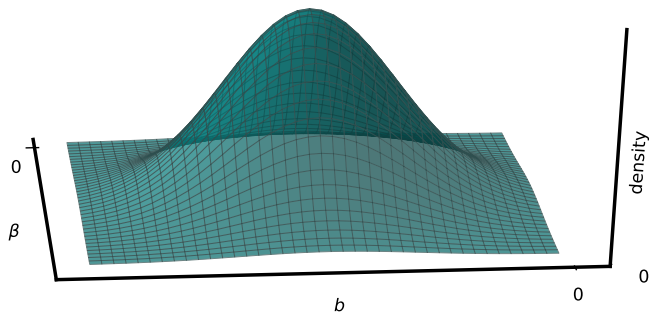
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- b : penalized parts with a proper (Gaussian) prior
 $\dim(b_j) = \text{rank}(K_j)$

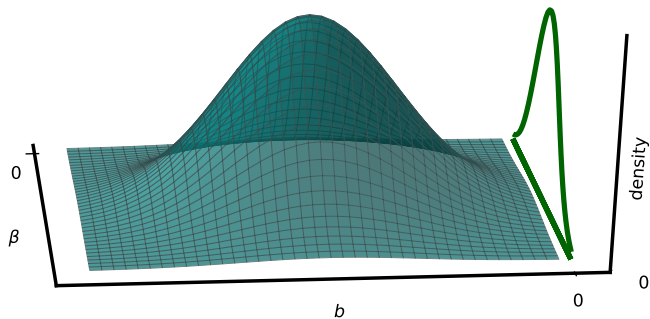
Mixed Model Representation

unpenalized likelihood



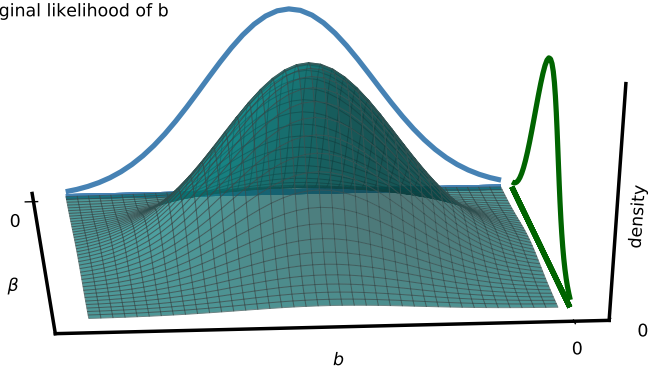
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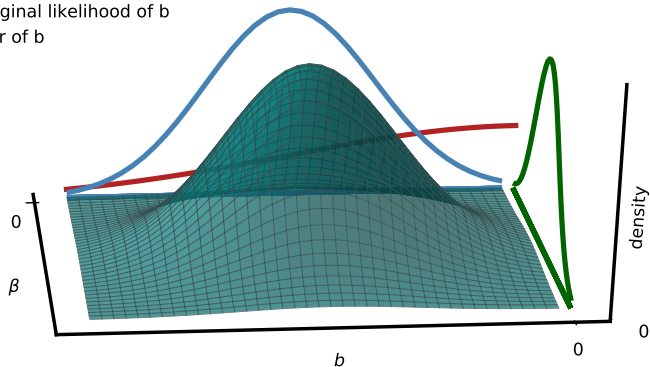
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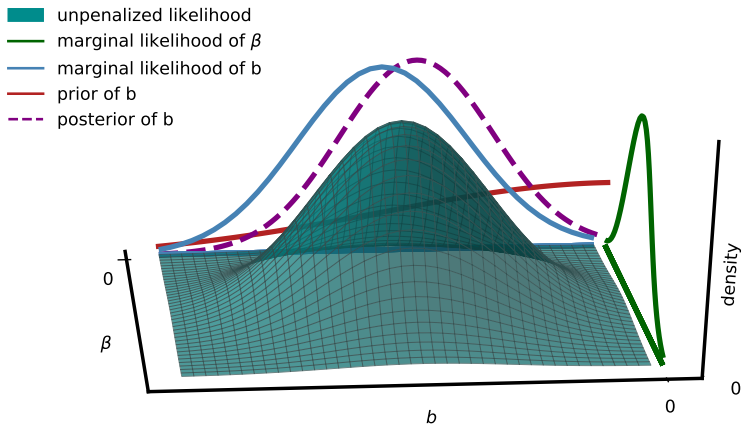


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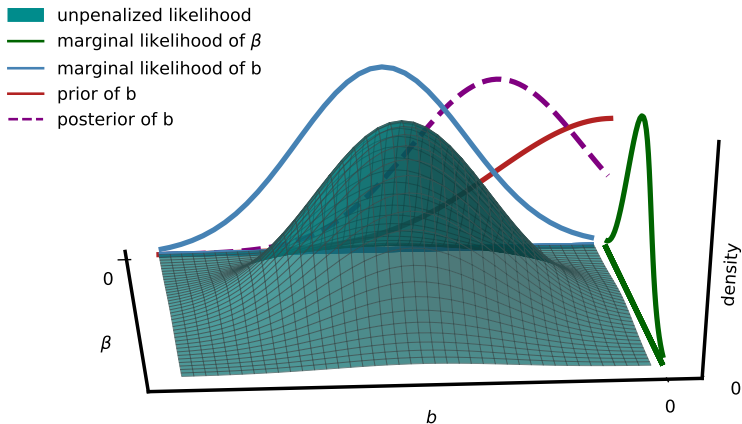
- unpenalized likelihood
- marginal likelihood of β
- marginal likelihood of b
- prior of b



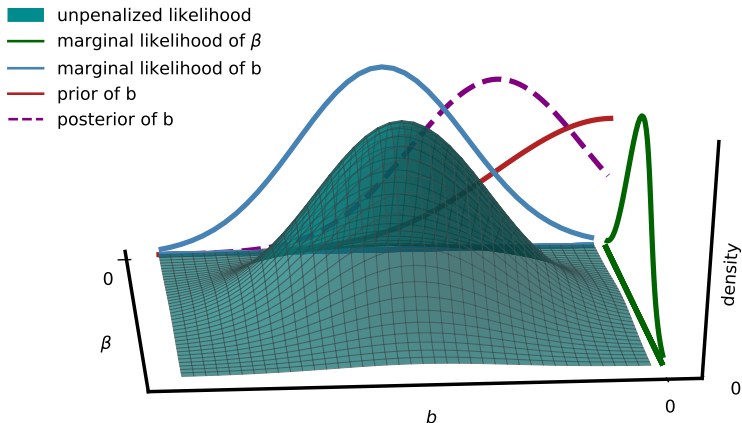
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The lower the prior variance, the higher the penalty!

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

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

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

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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 : $\tilde{Z}_j^T K_j \tilde{Z}_j = I_{k_j}$

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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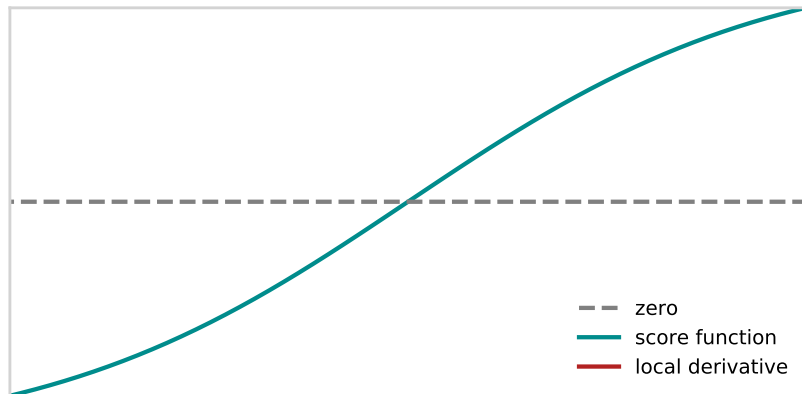
Mixed Model equations:

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

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

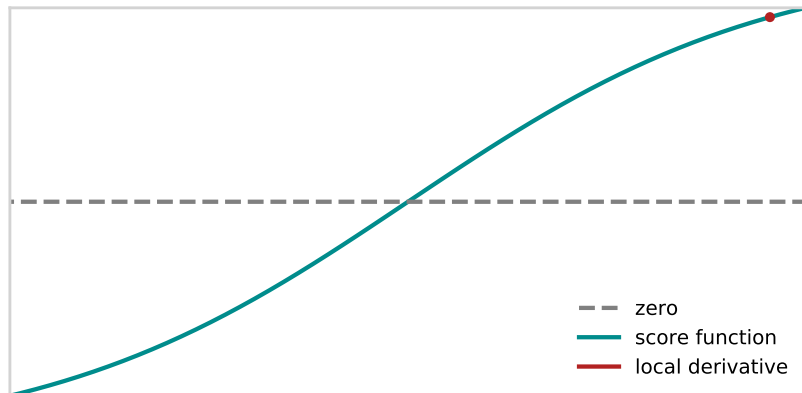
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



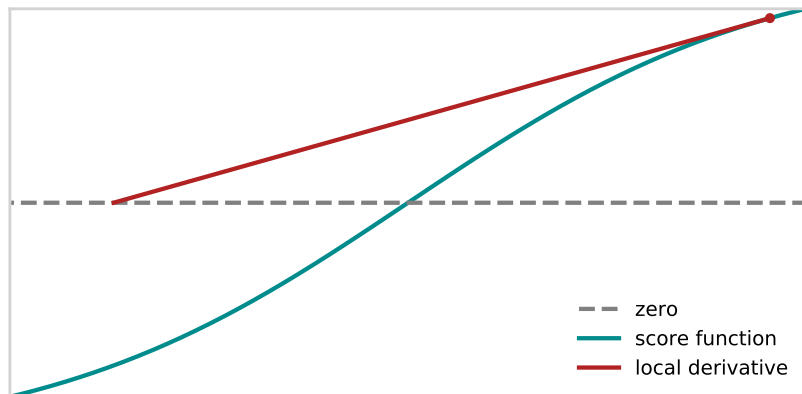
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



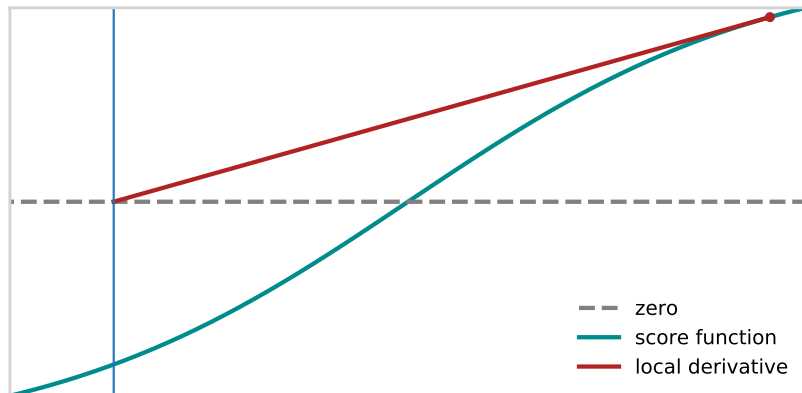
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



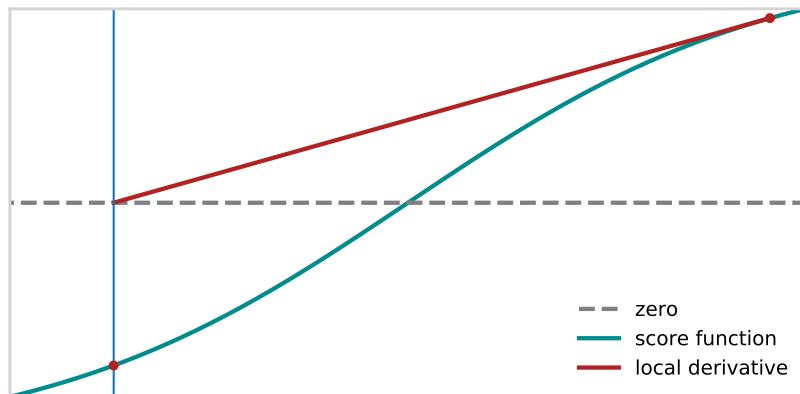
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



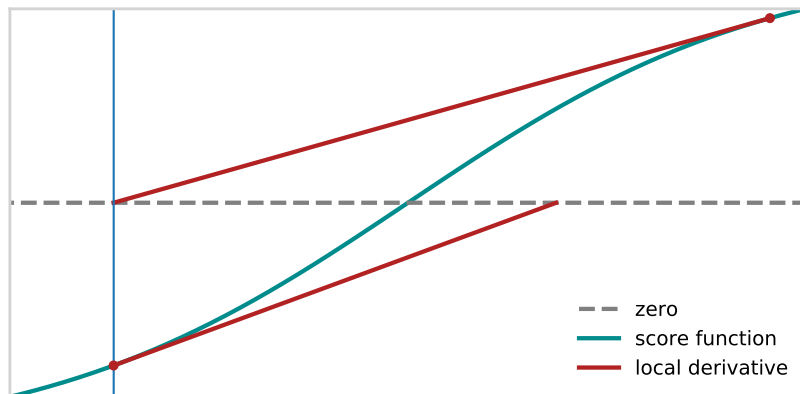
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



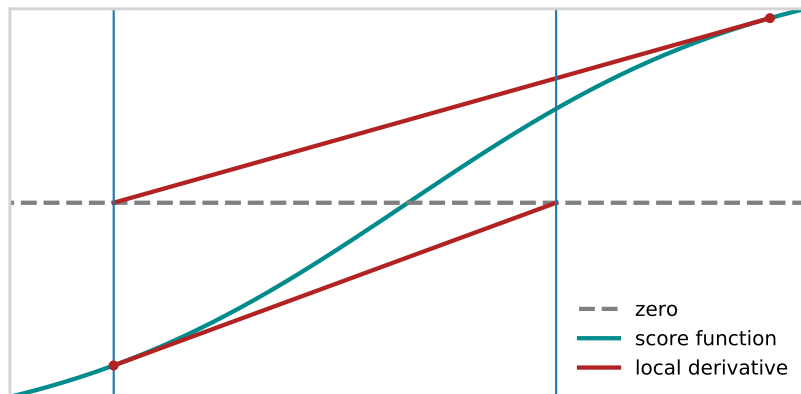
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



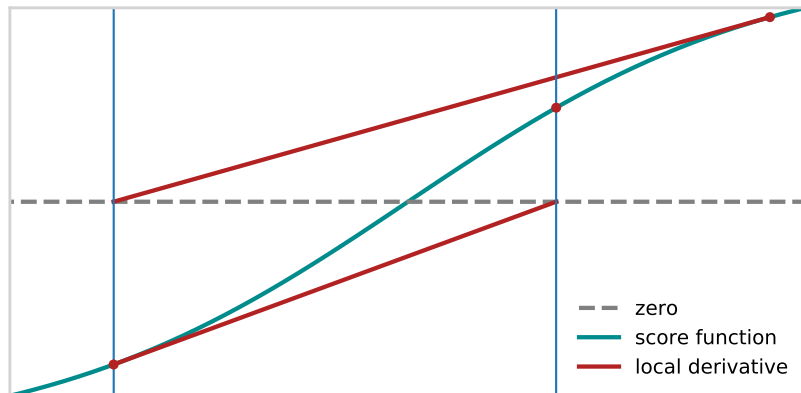
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



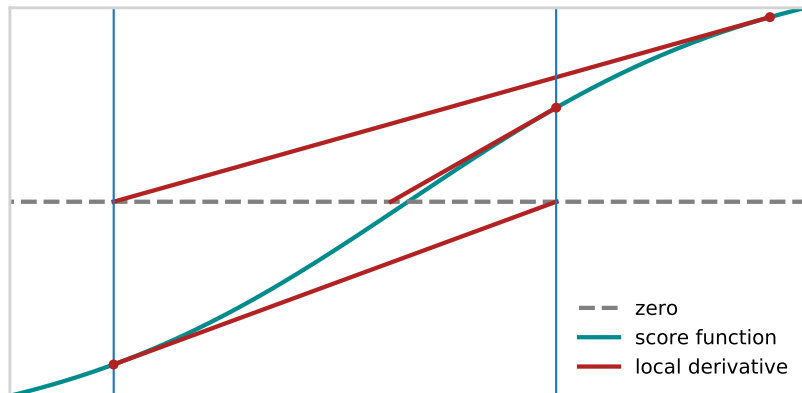
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



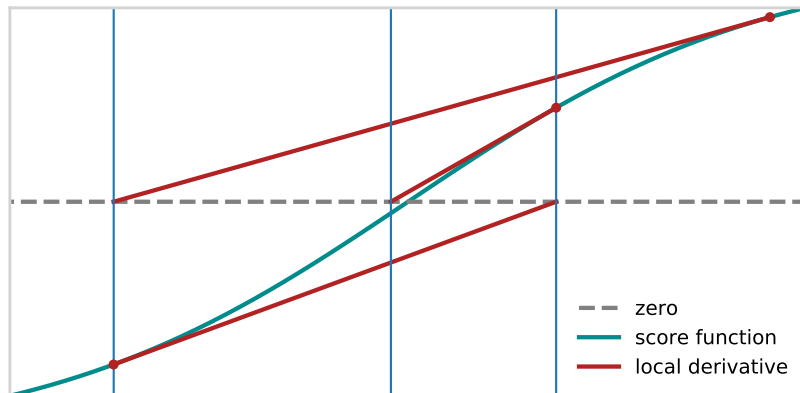
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



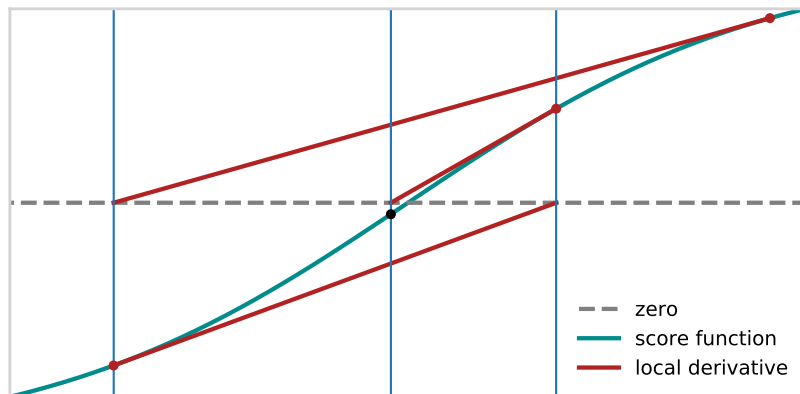
Variance Estimates $\hat{\sigma}^2$ and $\hat{\tau}^2$

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



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

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



Nested REML estimation

- **Estimate β and b :**

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

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

Solve with penalized iteratively re-weighted least squares & Newton

- **Estimate the variance components τ^2 and σ^2 :**

$$\vartheta^{(k+1)} = \vartheta^{(k)} + F^*(\vartheta^{(k)})^{-1} s^*(\vartheta^{(k)})$$

Applications

Comparison of Mixed Model Approach

Fully Bayesian approach (MCMC)

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

Prediction error methods (AIC, GCV)

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

Prospect





GLM

Non-spline semiparametric regression

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: $\lambda \propto \frac{1}{\tau^2}$
- For good results in mixed model inference, the **penalty term** has to be estimated in a **nested iteration** setup with the other parameters.

References

-  Fahrmeir, L., Kneib, T., Lang, S., & Marx, B. (2006). *Regression – Models, Methods and Applications*. Springer-Verlag Berlin Heidelberg.
-  Kneib, T. (2006). *Doctoral Thesis*, LMU Munich.
Mixed model based inference in structured additive regression.
-  Wood, S. N. (2017). *Generalized Additive Models: An Introduction with R*. Chapman and Hall/CRC.
-  Wood, S. N. (2011). *J. R. Statist. Soc. B*, 73: 3–36.
Fast stable REML and ML estimation of semiparametric GLMs.

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

Recap: Conditions

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

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 $L_j = \Gamma \Lambda_j^{1/2}$

Variance Estimates

Maximum Likelihood (ML)

- uses marginal likelihood $y|\beta \sim N(X\beta, \Sigma)$
 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

Restricted ML (REML)

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