

# Representing Additive Models as Mixed Models

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LMU Seminar: Mixed and Semiparametric Models

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# Truncated Power Basis

univariate:

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

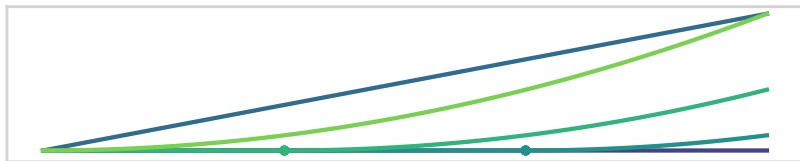
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univariate and quadratic with two knots:

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



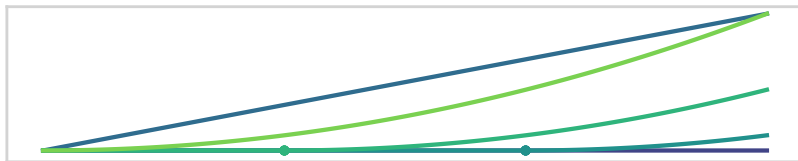
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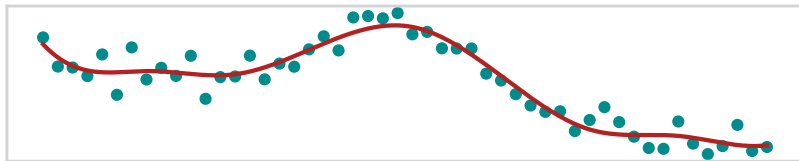
$$y = \overbrace{\theta_0 + \theta_1 x + \theta_2 x^2}^{\text{fixed effects}} + \overbrace{\theta_{21} (x - \kappa_1)_+^2 + \theta_{22} (x - \kappa_2)_+^2}^{\text{random effects: depend on } i} + \epsilon$$



# Additive Models

Semiparametric regression:

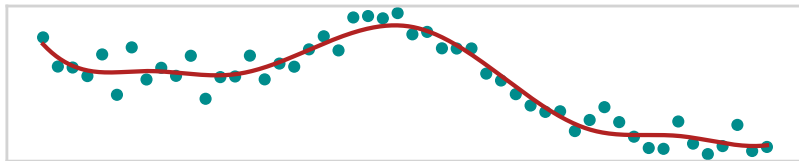
$$\hat{y}_i = f(\nu_i) + u_i^T \gamma$$



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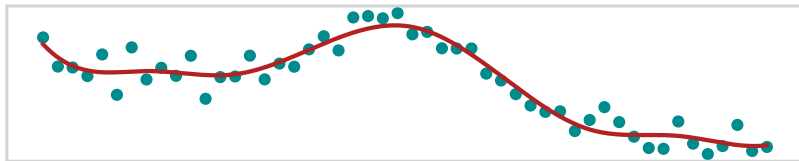
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Semiparametric regression:

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In matrix notation:

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

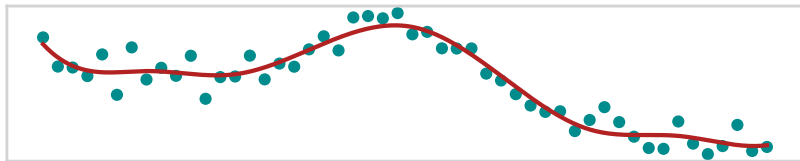


# Additive Models

Semiparametric regression:

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

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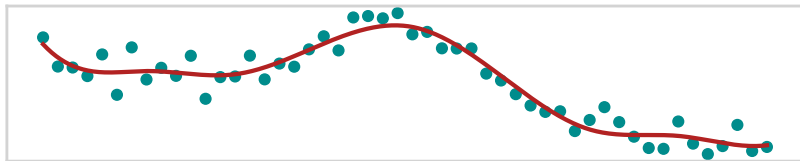
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In matrix notation:

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



## Splines

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

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

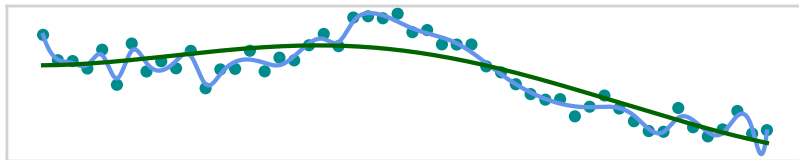


# Roughness Penalty

Penalized Regression Spline:

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

Control wiggleness (bias-variance tradeoff):

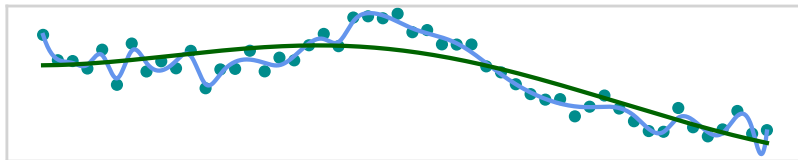


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e. g. first order differences  $\xi^T K \xi = \sum (\xi_{k+1} - \xi_k)^2$ :

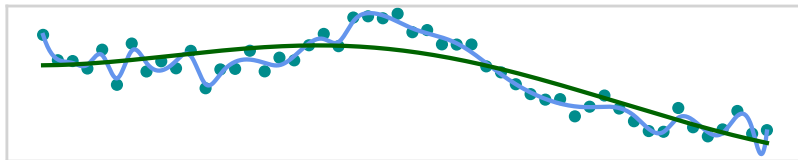


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Problem: How to choose  $\lambda$ ?



# 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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- **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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- Maximum Likelihood for  $\tau_j^2$  (so far treated as fixed):

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

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

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- $\beta$ : non-penalized parts with a flat prior  
 $\dim(\beta_j) = \dim(\xi_j) - \text{rank}(K_j)$

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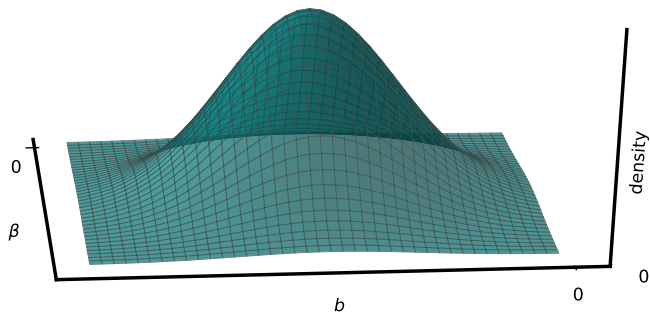
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- $\beta$ : non-penalized parts with a flat prior  
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- $b$ : penalized parts with a proper (Gaussian) prior  
 $\dim(b_j) = \text{rank}(K_j)$



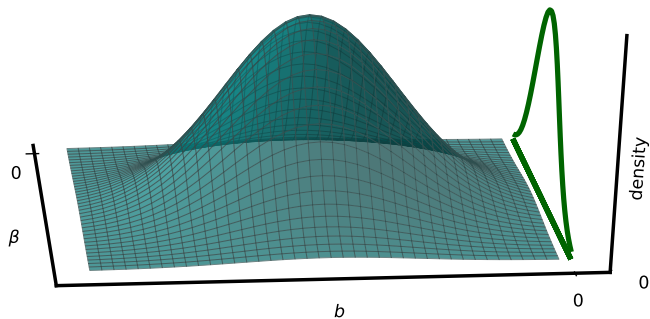
# Mixed Model Representation

unpenalized likelihood



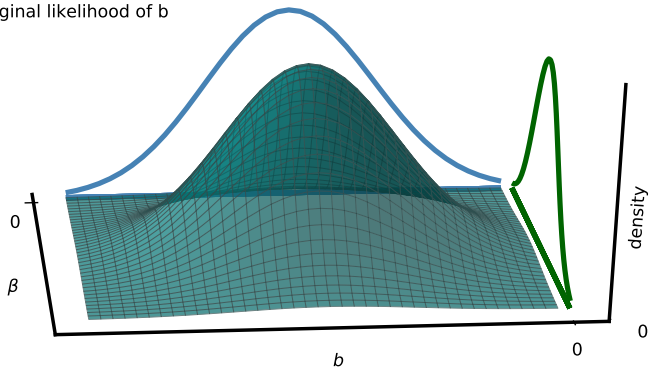
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- unpenalized likelihood
- marginal likelihood of  $\beta$



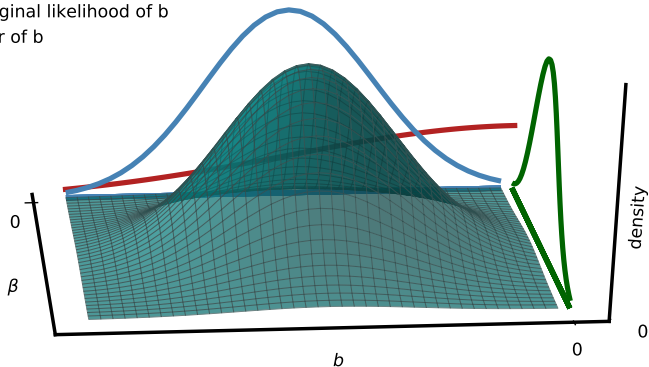
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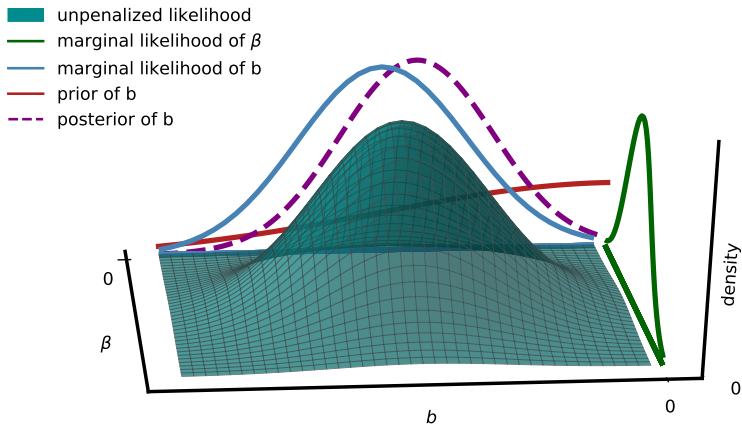


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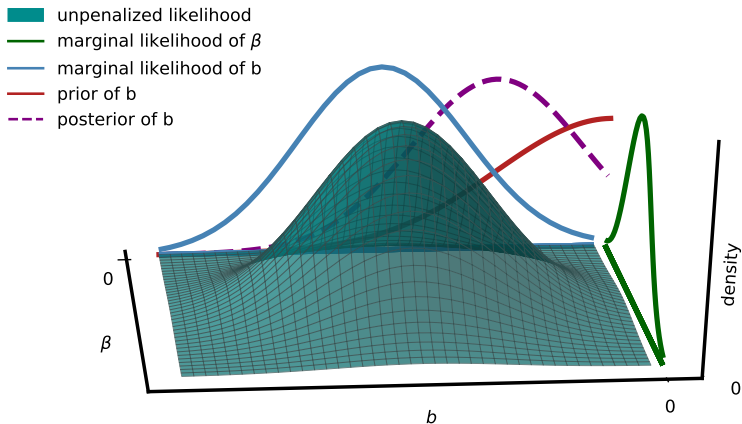
- unpenalized likelihood
- marginal likelihood of  $\beta$
- marginal likelihood of  $b$
- prior of  $b$



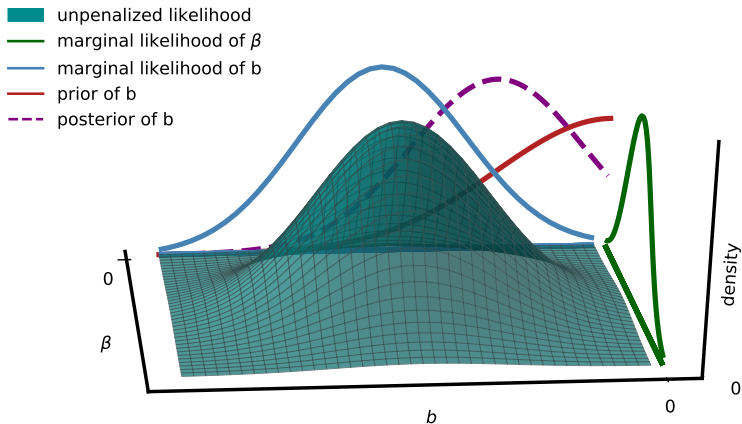
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The lower the prior variance, the higher the penalty!

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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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3.  $\beta_j$  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:

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



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

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  $\beta$  and  $b$  simultaneously based on known  $\sigma^2$  and  $\tau^2$ .

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

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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 (partial) marginal distribution  $y \sim N(X\beta, \Sigma)$ 
  1. Derive  $\hat{\beta}$  analytically
  2. Plug in to get profile likelihood for  $\tau^2$  and  $\sigma^2$
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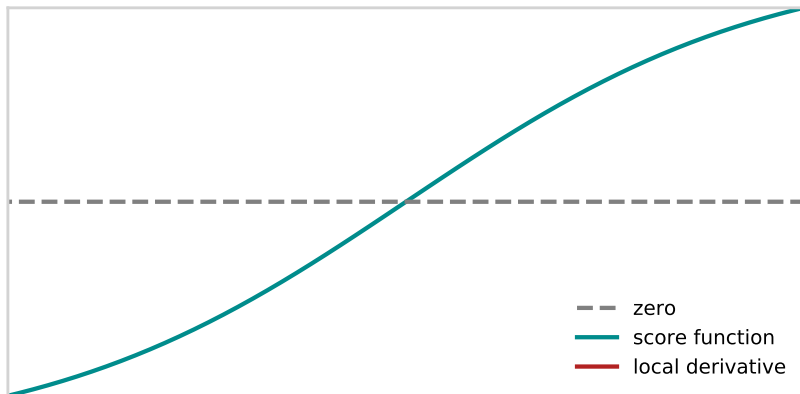
## Restricted ML (integrate $b$ and $\beta$ out)

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



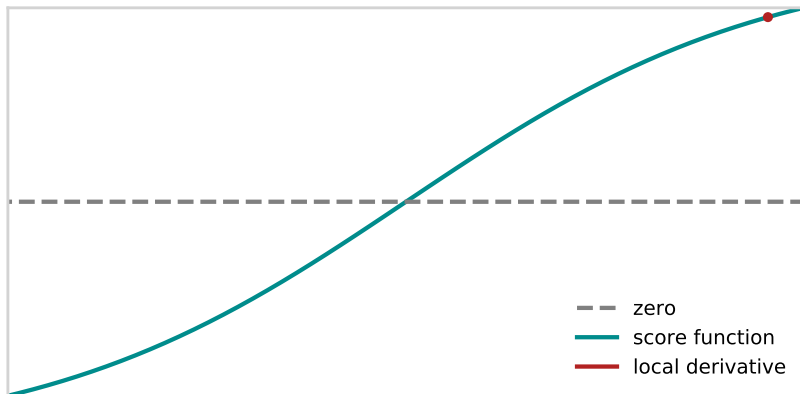
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Maximize the restricted likelihood (REML) using Newton-Raphson:



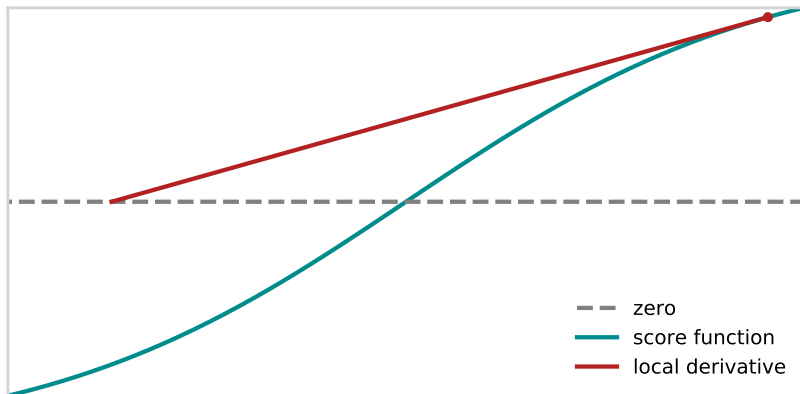
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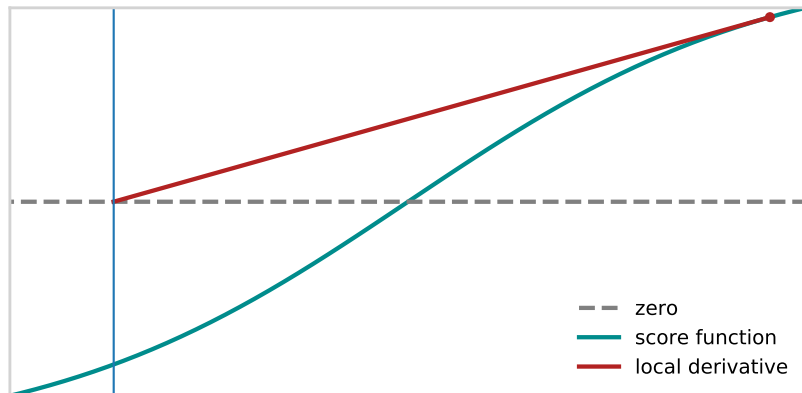
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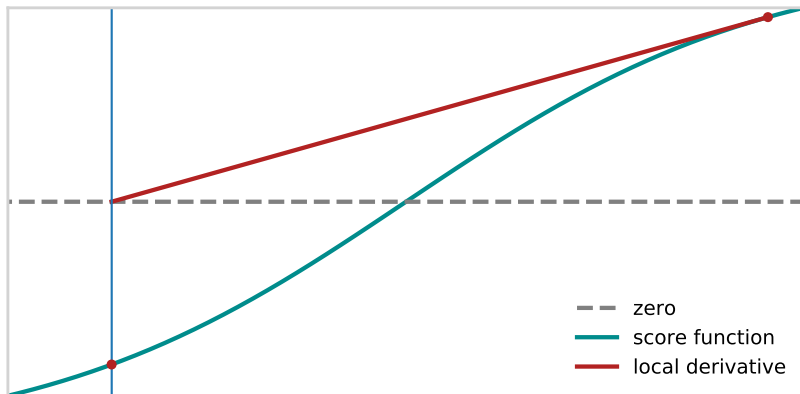
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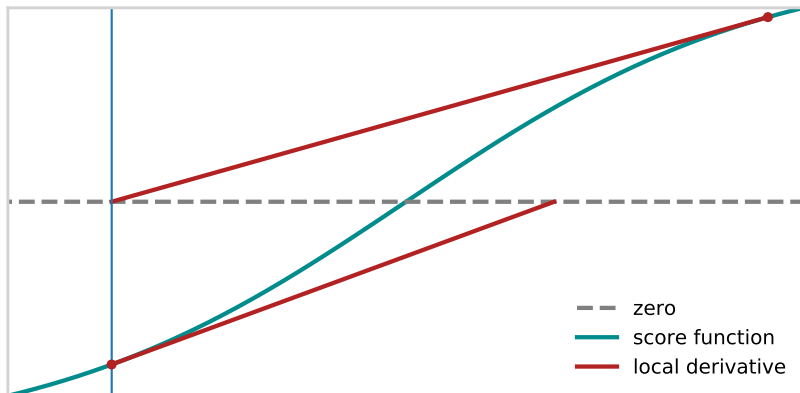
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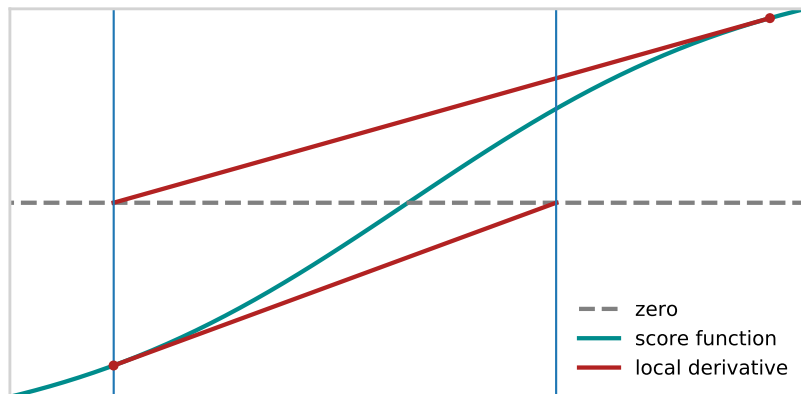
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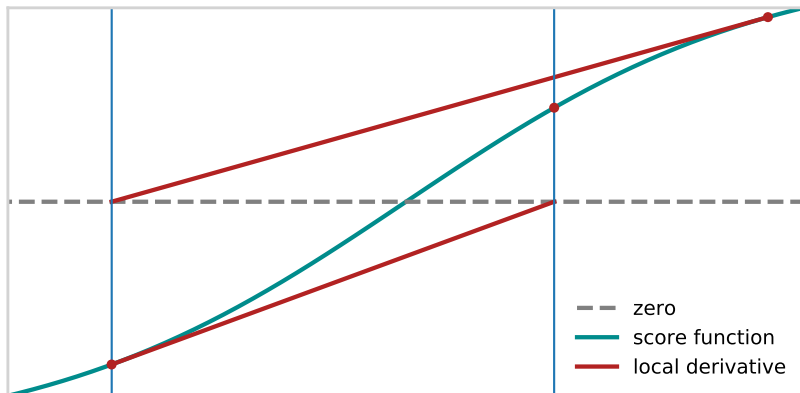
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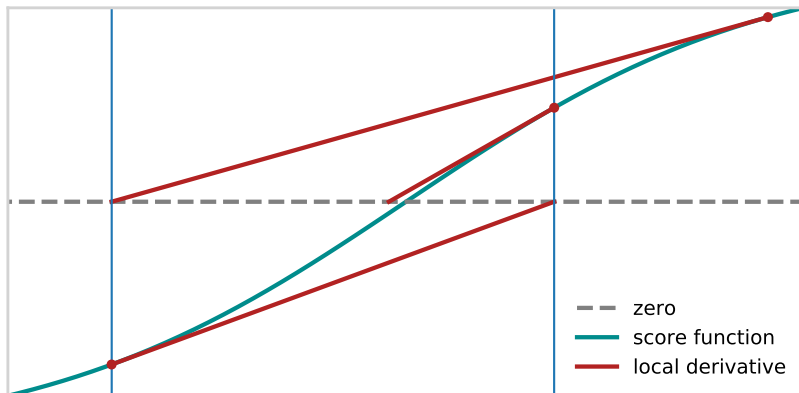
Maximize the restricted likelihood (REML) using Newton-Raphson:





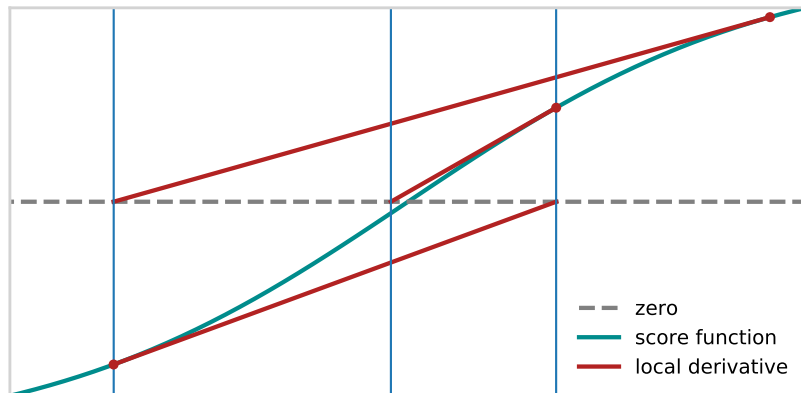
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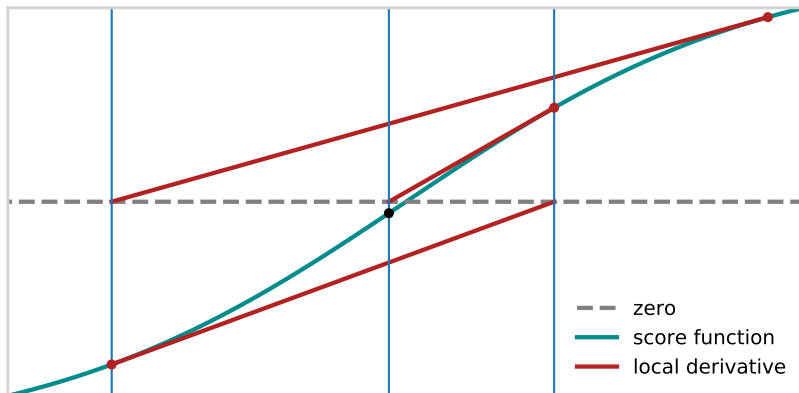
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# (RE)ML estimation

## Single iterations (old)

1. Update  $\hat{\beta}$  and  $\hat{b}$  given the current  $\hat{\lambda}$
2. Update  $\hat{\lambda}$  using Fisher-Scoring (or Newton-Raphson)
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## Nested iterations (new)

1. **Estimate the penalty  $\lambda$ :**  
Using Newton-Raphson
  - For each  $\hat{\lambda}$ : Get estimates for  $\beta$  and  $b$ :  
Solve with penalized iteratively re-weighted least squares (PIRLS) and Newton-Raphson
2. **Iterate until convergence**

# Comparison of Mixed Model Approach

## Fully Bayesian approach (MCMC)

- + no reparameterization needed
- identifiability problems less detectable
- 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
- *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:  $\lambda \propto \frac{1}{\tau^2}$
- For good results in mixed model inference, the **penalty term** has to be estimated in a **nested iteration** setup with the other parameters.

## References

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