Representing Additive Models as Mixed Models

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LMU Seminar: Mixed and Semiparametric Models

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Truncated Power Basis

univariate:

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

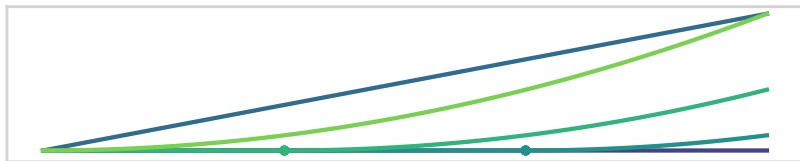## Truncated Power Basis

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univariate and quadratic with two knots:

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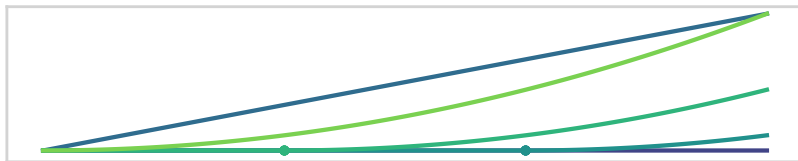
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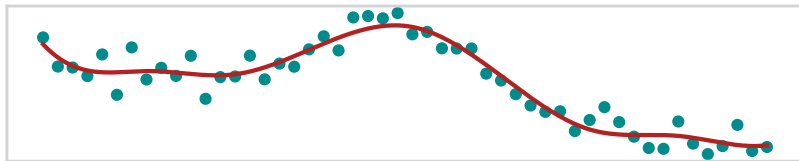
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Introduction
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Recap
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Representation
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Inference
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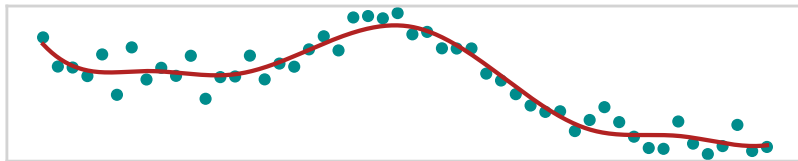
Conclusion
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Additive Models

Semiparametric regression:

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

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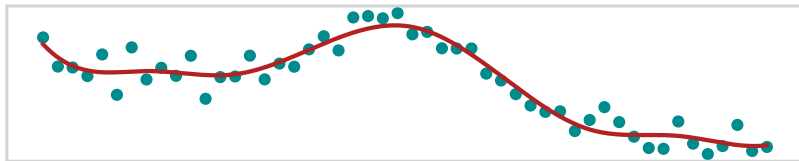Introduction
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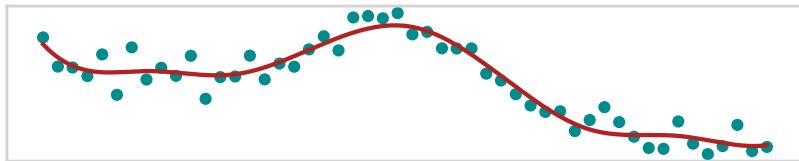
In matrix notation:

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

Additive Models

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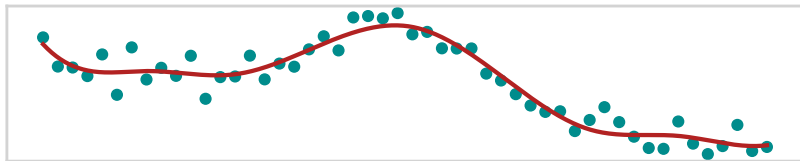$$\hat{y} = V_1\xi_1 + ... + V_p\xi_p + U\gamma = \sum_{j=1}^{p} V_j\xi_j + U\gamma$$

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, ...
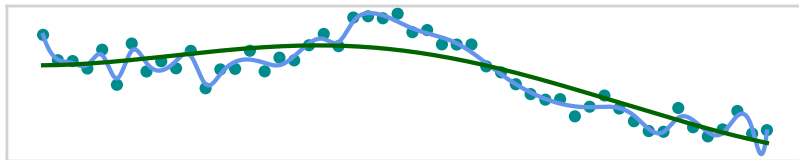
Roughness Penalty

Penalized Regression Spline:

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

Control wiggliness (bias-variance tradeoff):

Roughness Penalty

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e. g. first order differences $\xi^T K \xi = \sum (\xi_{k+1} - \xi_k)^2$:
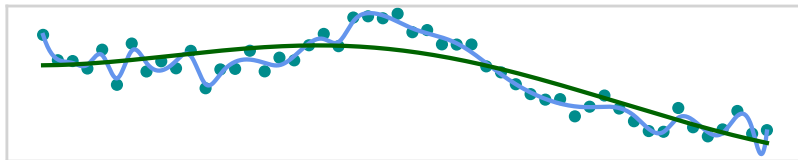
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Problem: How to choose λ?
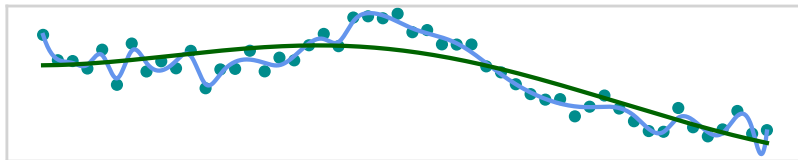
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- **Idea:** Use Mixed Model inference: $y = \sum_{j=1}^{p} \underbrace{V_p \xi_p}_{\text{random effects}} + \overbrace{U\gamma}^{\text{fixed effects}} + \epsilon$

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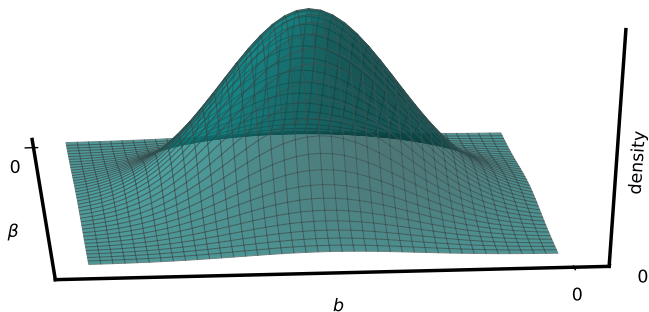The Gaussian prior $p(\xi_j | \tau_j^2) \propto \exp\left(-\frac{1}{2\tau_j^2} \xi_j^T K_j \xi_j\right)$ is improper.

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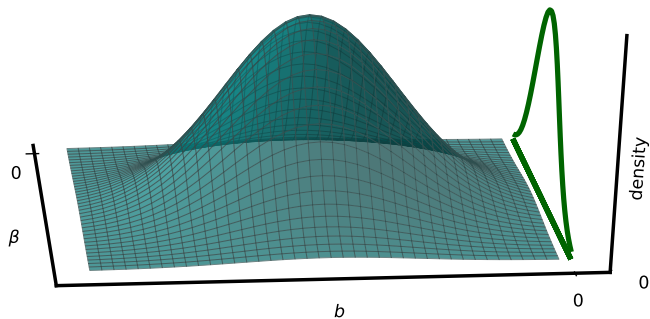 $\dim(b_j) = \text{rank}(K_j)$

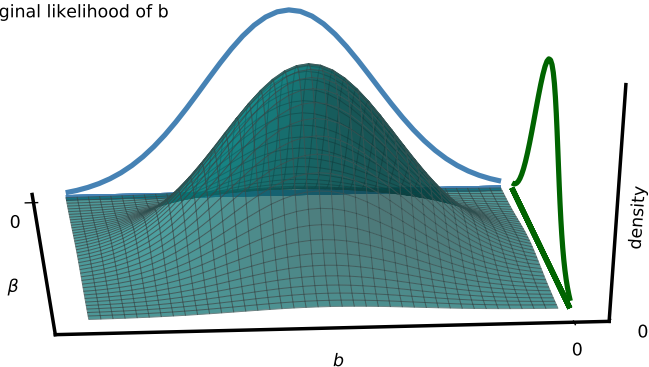# Mixed Model Representation

■ unpenalized likelihood

Introduction
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Recap
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Representation
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Inference
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Conclusion
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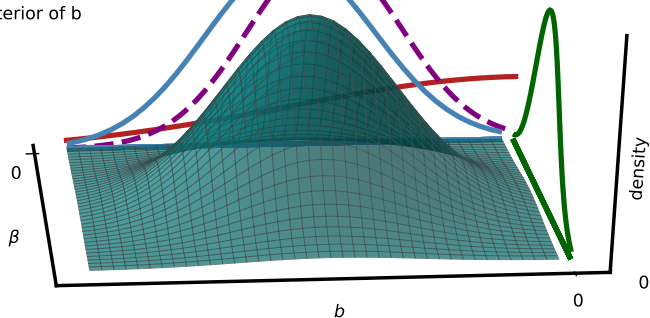oo●oo

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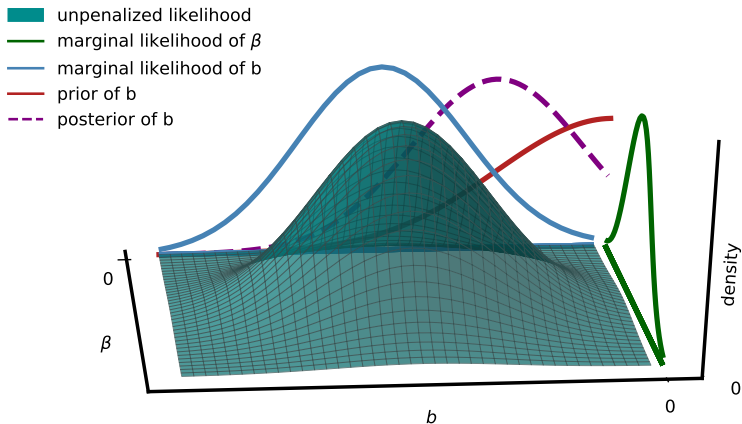oooo

Conclusion
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Mixed Model Representation

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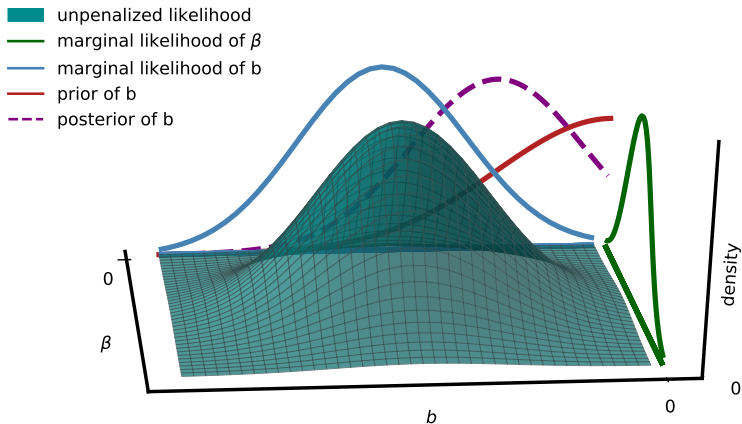- marginal likelihood of b
- prior of b
- posterior of b

The lower the prior variance, the higher the penalty!

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$$\beta := (\beta_1^T, ..., \beta_p^T, \gamma^T)$$
$$b := (b_1^T, ..., b_p^T)$$
$$Z := V_j \tilde{Z}_j$$
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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: $\tilde{Z}_j^T K_j \tilde{Z}_j = I_{k_j}$

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log-Prior:

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

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 $\hat{b}$

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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 $Q = \text{blockdiag}(\tau_1^2 I_{k1}, ..., \tau_p^2 I_{kp})$

Variance Estimates
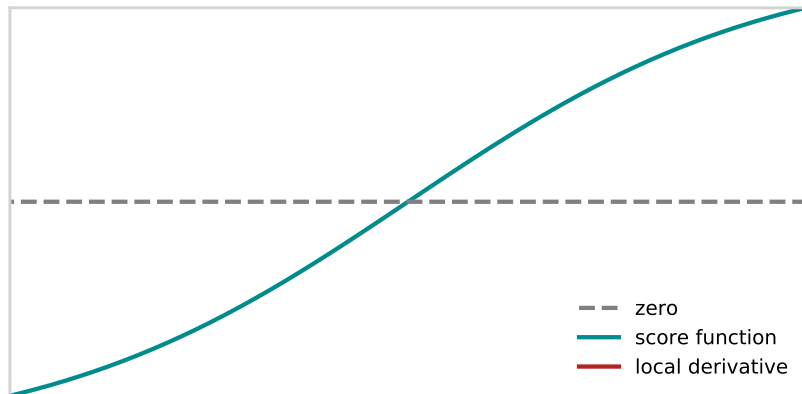
Maximum Likelihood (integrate b out)

- uses (partialy) 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 $\hat{\tau}^2$

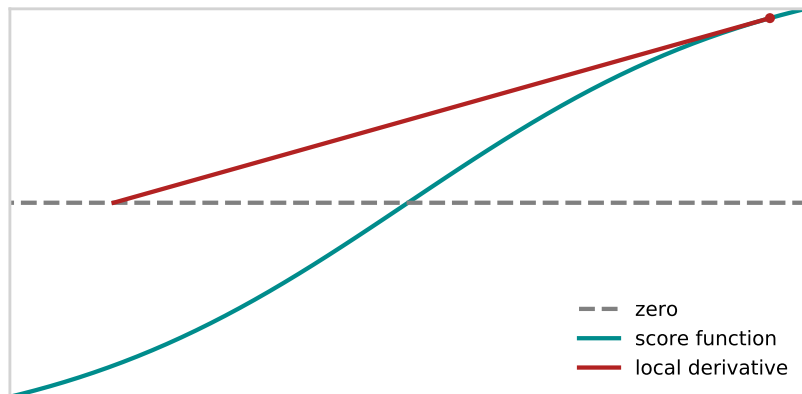Maximize the restricted likelihood (REML) using Newton-Raphson:

- - - zero
— score function
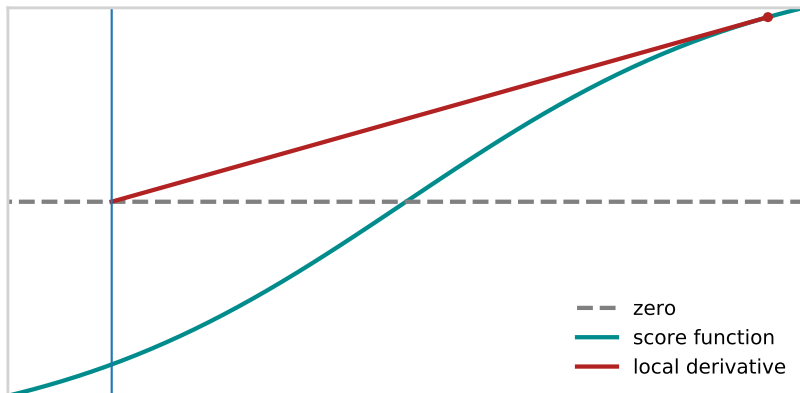— local derivative

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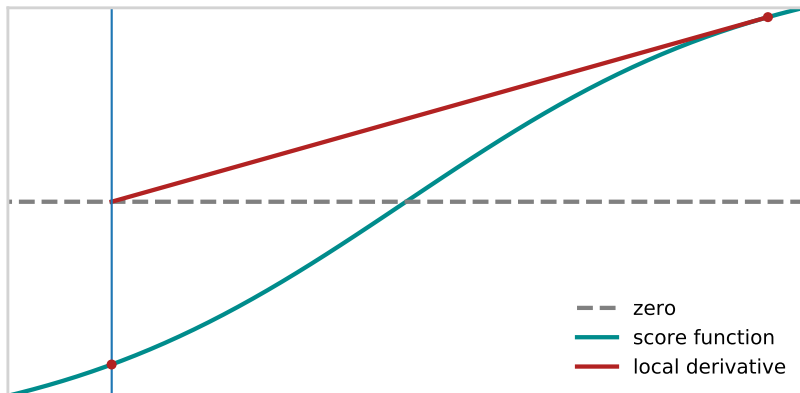— local derivative

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

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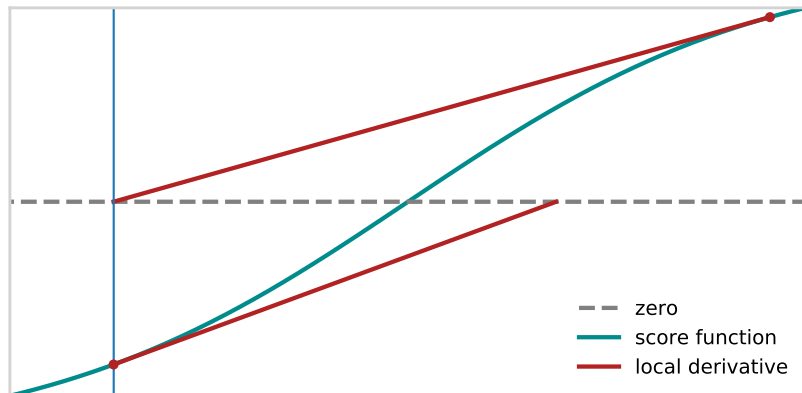local derivative

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Introduction
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Recap
oooo

Representation
ooooo

Inference
oo●o

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

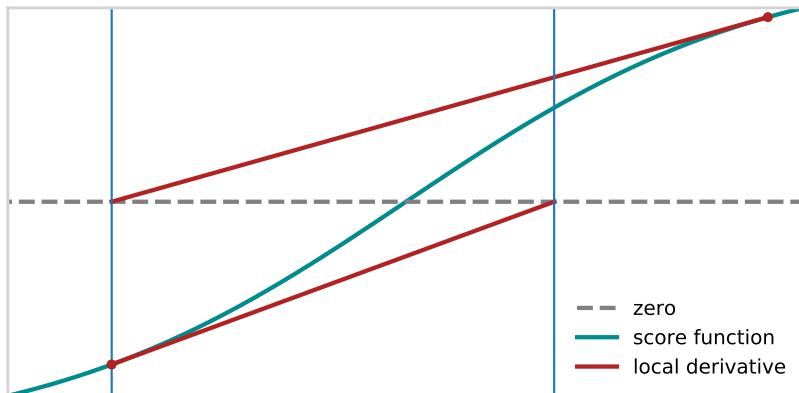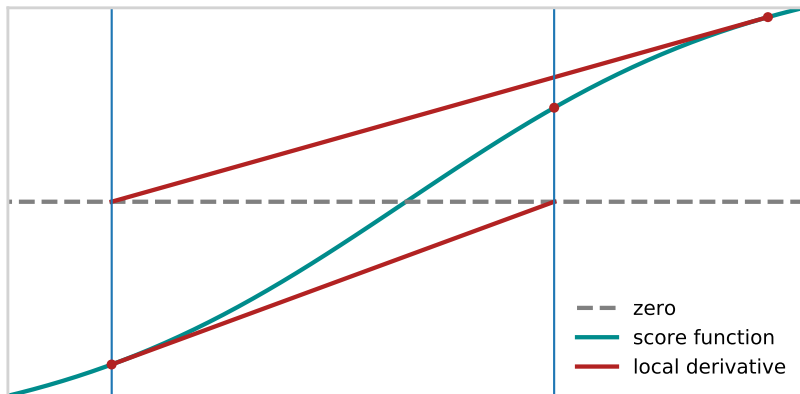Maximize the restricted likelihood (REML) using Newton-Raphson:

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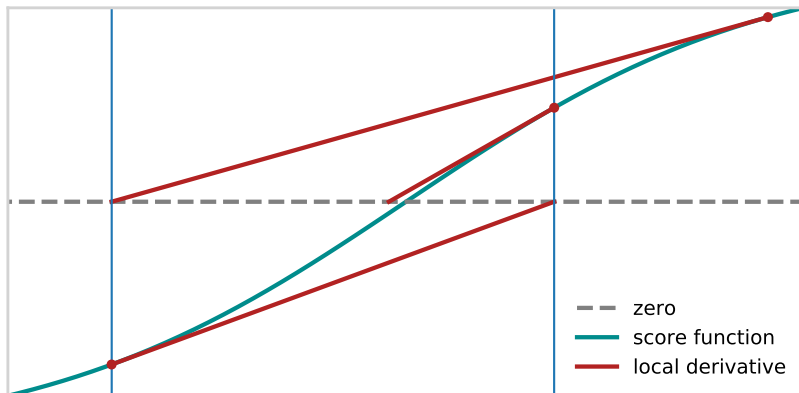

- - - zero
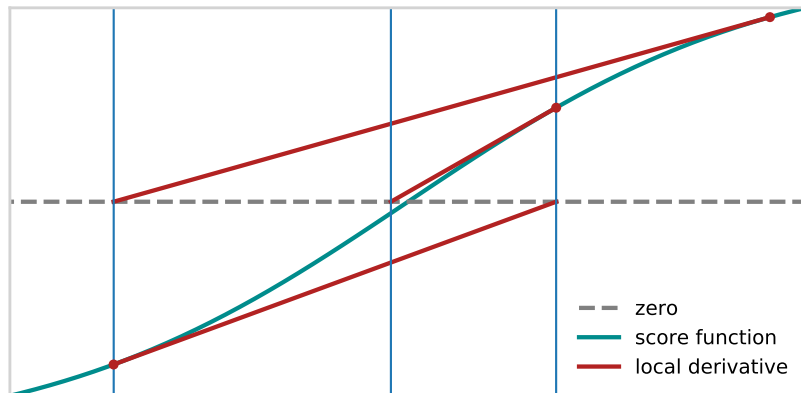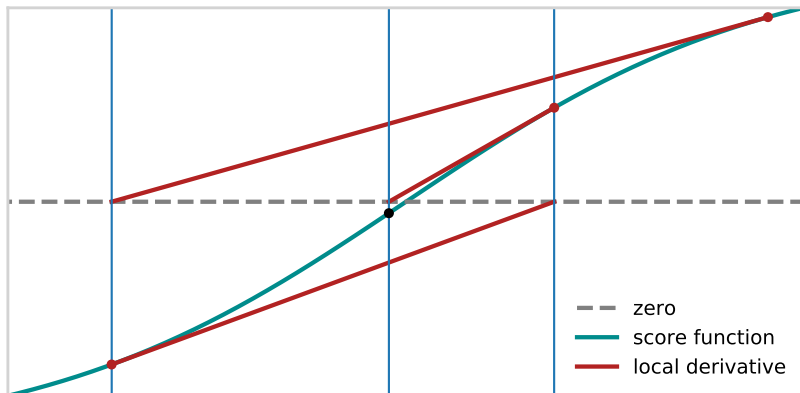— score function
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(RE)ML estimation

Single iterations (old)

1. Update $\hat{\beta}$ and $\hat{b}$ given the current λ
2. Update $\hat{\lambda}$ using Fisher-Scoring (or Newton-Raphson)
3. Iterate until convergence

(RE)ML estimation

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Nested iterations (new)

1. **Estimate the penalty λ:**
   Using Newton-Raphson

   - For each $\hat{\lambda}$: Get estimates for β 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.

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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: $K_j = \Gamma_j \Lambda_j \Gamma^T$, so $L_j = \Gamma \Lambda_j^{1/2}$