Chapter 1

GCV

1.1 GCV-I-derivative

$\frac{dGCV}{d\lambda}(\lambda) = \frac{d(s\frac{SS_{res}(\lambda)}{dor^2(\lambda)})}{d\lambda} = s(\frac{dSS_{res}}{d\lambda}\frac{1}{dor^2} + SS_{res}\frac{d(dor^{-2})}{d\lambda})$

$[1] = \frac{dSS_{res}}{d\lambda} = \frac{d(<\hat{\varepsilon},\hat{\varepsilon}>)}{d\lambda} = 2 < \frac{d\hat{\varepsilon}}{d\lambda}, \hat{\varepsilon} >= 2 < \frac{d((\boldsymbol{Q}-\boldsymbol{QS})\boldsymbol{z})}{d\lambda}, \hat{\varepsilon} >= -2 < \boldsymbol{Q}\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\varepsilon} > \overset{\boldsymbol{Q}\in Sym}{=}$
$-2 < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \boldsymbol{Q}\hat{\varepsilon} > \overset{\boldsymbol{Q}^2=\boldsymbol{Q}}{=} -2 < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\varepsilon} >$

$[2] = \frac{d(dor^{-2})}{d\lambda} = -2\frac{1}{dor^3}\frac{d(dor)}{d\lambda} = -2\frac{1}{dor^3}\frac{d(s-q-tr(\boldsymbol{S}))}{d\lambda} = 2\frac{1}{dor^3}tr(\frac{d\boldsymbol{S}}{d\lambda})$

$\implies \frac{dGCV}{d\lambda}(\lambda) = s(- < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\varepsilon} > \frac{2}{dor^2} + SS_{res}\frac{2}{dor^3}tr(\frac{d\boldsymbol{S}}{d\lambda})) = \frac{2s}{dor^2}(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}) + a)$

1.1.1 Fundamental matrices

1. $\mathbf{R} = \mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1}$
2. $\mathbf{T} = \boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1} = \boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R}$
3. $\mathbf{V} = (\boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1})^{-1}\boldsymbol{\Psi}^t\mathbf{Q} = \boldsymbol{T}^{-1}\boldsymbol{\Psi}^t\mathbf{Q}$
4. $\mathbf{S} = \boldsymbol{\Psi}(\boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1})^{-1}\boldsymbol{\Psi}^t\mathbf{Q} = \boldsymbol{\Psi}\boldsymbol{V}$
5. $\frac{d\boldsymbol{S}}{d\lambda} = -\boldsymbol{\Psi}(\boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1})^{-1}\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1}(\boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1})^{-1}\boldsymbol{\Psi}^t\mathbf{Q}$
$= -\boldsymbol{\Psi}\mathbf{T}^{-1}\mathbf{R}\mathbf{V} = -\boldsymbol{\Psi}\mathbf{K}\mathbf{V} = -\boldsymbol{\Psi}\mathbf{F}$

Useful stored factors

1. $\mathbf{K} = \mathbf{T}^{-1}\mathbf{R}$
2. $\mathbf{F} = \mathbf{K}\mathbf{V}$
3. $\mathbf{t} = \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}$
4. $a = - < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\varepsilon} >= - < \mathbf{t}, \hat{\varepsilon} >$

1.2 GCV-II-derivative

$\frac{d^2GCV}{d\lambda^2}(\lambda) = 2s\frac{d(dor^{-2}(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda})-<\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z},\hat{\boldsymbol{\varepsilon}}>))}{d\lambda}$

$[1] = \frac{d(dor^{-2})}{d\lambda}(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda})- < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} >) = 2\frac{1}{dor^3}tr(\frac{d\boldsymbol{S}}{d\lambda})(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda})- < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} >)$

$[2] = \frac{1}{dor^2}\frac{d(\hat{\sigma}^2)}{d\lambda}tr(\frac{d\boldsymbol{S}}{d\lambda}) = \frac{1}{dor^2}\frac{\frac{d(SS_{res})}{d\lambda}dor - SS_{res}\frac{d(dor)}{d\lambda}}{dor^2}tr(\frac{d\boldsymbol{S}}{d\lambda}) = \frac{1}{dor^2}\frac{-2<\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z},\hat{\boldsymbol{\varepsilon}}>dor + SS_{res}tr(\frac{d\boldsymbol{S}}{d\lambda})}{dor^2}tr(\frac{d\boldsymbol{S}}{d\lambda}) = \frac{1}{dor^3}(-2 < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} > + \hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}))tr(\frac{d\boldsymbol{S}}{d\lambda})$

$[3] = \frac{1}{dor^2}\hat{\sigma}^2 tr(\frac{d^2\boldsymbol{S}}{d\lambda^2})$

$[4] = -\frac{1}{dor^2} < \frac{d^2\boldsymbol{S}}{d\lambda^2}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} >$

$[5] = -\frac{1}{dor^2} < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \frac{d\hat{\boldsymbol{\varepsilon}}}{d\lambda} >= \frac{1}{dor^2} < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \boldsymbol{Q}\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z} >$

$\Longrightarrow \frac{d^2GCV}{d\lambda^2}(\lambda) =$
$= \frac{2s}{dor^2}\{\frac{1}{dor}[3\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}) - 4 < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} >]tr(\frac{d\boldsymbol{S}}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2\boldsymbol{S}}{d\lambda^2}) + < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \boldsymbol{Q}\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z} > - < \frac{d^2\boldsymbol{S}}{d\lambda^2}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} >\} =$
$= \frac{2s}{dor^2}\{\frac{1}{dor}[3\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}) + 4a]tr(\frac{d\boldsymbol{S}}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2\boldsymbol{S}}{d\lambda^2}) + b + c\}$

1.2.1 Fundamental matrices

1. $\frac{d^2\boldsymbol{S}}{d\lambda^2} = 2\boldsymbol{\Psi}[(\boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1})^{-1}\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1}]^2(\boldsymbol{\Psi}^t\mathbf{Q}\boldsymbol{\Psi} + \lambda\mathbf{R_1}^t\mathbf{R_0}^{-1}\mathbf{R_1})^{-1}\boldsymbol{\Psi}^t\mathbf{Q}$
   $= 2\boldsymbol{\Psi}(\mathbf{T}^{-1}\mathbf{R})^2\mathbf{V} = 2\boldsymbol{\Psi}\mathbf{K}^2\mathbf{V} = 2\boldsymbol{\Psi}\mathbf{K}\mathbf{F}$

Useful stored factors

1. $b =< \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z}, \boldsymbol{Q}\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z} >=< \boldsymbol{t}, \boldsymbol{Q}\boldsymbol{t} >$
2. $c = - < \frac{d^2\boldsymbol{S}}{d\lambda^2}\boldsymbol{z}, \hat{\boldsymbol{\varepsilon}} >$

Chapter 2

Forced GCV

2.1 GCV-I-derivative

$\frac{dGCV}{d\lambda}(\lambda) = \frac{d(s\frac{SS_{res}(\lambda)}{dor^2(\lambda)})}{d\lambda} = s(\frac{dSS_{res}}{d\lambda}\frac{1}{dor^2} + SS_{res}\frac{d(dor^{-2})}{d\lambda})$

$[1] = \frac{dSS_{res}}{d\lambda} = \frac{d(<\hat{\varepsilon},\hat{\varepsilon}>)}{d\lambda} = 2 < \frac{d\hat{\boldsymbol{\varepsilon}}}{d\lambda}, \hat{\boldsymbol{\varepsilon}} >= 2 < \frac{d((\boldsymbol{Q}-\boldsymbol{QS})\boldsymbol{z}-\mathbf{r})}{d\lambda}, \hat{\boldsymbol{\varepsilon}} >= -2 < \boldsymbol{Q}(\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z} + \frac{d\boldsymbol{s}}{d\lambda}), \hat{\boldsymbol{\varepsilon}} > \overset{\boldsymbol{Q}\in Sym}{=} -2 < \frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z} + \frac{d\boldsymbol{s}}{d\lambda}, \boldsymbol{Q}\hat{\varepsilon} > \overset{\boldsymbol{Q}^2=\boldsymbol{Q}}{=} 2 < \boldsymbol{\Psi h} - \boldsymbol{t}, \hat{\boldsymbol{\varepsilon}} >= 2a$

$[2] = \frac{d(dor^{-2})}{d\lambda} = -2\frac{1}{dor^3}\frac{d(dor)}{d\lambda} = -2\frac{1}{dor^3}\frac{d(s-q-tr(\boldsymbol{S}))}{d\lambda} = 2\frac{1}{dor^3}tr(\frac{d\boldsymbol{S}}{d\lambda})$

$\implies \frac{dGCV}{d\lambda}(\lambda) = s(\frac{2a}{dor^2} + SS_{res}\frac{2}{dor^3}tr(\frac{d\boldsymbol{S}}{d\lambda})) = \frac{2s}{dor^2}(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}) + a)$

Useful side computations

1. $\mathbf{s} = \lambda\boldsymbol{\Psi}\mathbf{T}^{-1}\mathbf{R}_1^T\mathbf{R}_0^{-1}\mathbf{u} = \lambda\boldsymbol{\Psi}\mathbf{g}$
2. $\mathbf{r} = \lambda\mathbf{Q}\boldsymbol{\Psi}\mathbf{T}^{-1}\mathbf{R}_1^T\mathbf{R}_0^{-1}\mathbf{u} = \lambda\mathbf{Q}\boldsymbol{\Psi}\mathbf{g} = \mathbf{Qs}$
3. $\frac{d\boldsymbol{s}}{d\lambda} = \boldsymbol{\Psi}\mathbf{g} - \lambda\boldsymbol{\Psi}\mathbf{T}^{-1}\mathbf{R}\mathbf{T}^{-1}\mathbf{R}_1^T\mathbf{R}_0^{-1}\mathbf{u} = \boldsymbol{\Psi}\mathbf{g} - \lambda\boldsymbol{\Psi}\mathbf{K}\mathbf{g} = \boldsymbol{\Psi}(\mathbf{I} - \lambda\mathbf{K})\mathbf{g}$

Useful stored factors

1. $\mathbf{f} = \mathbf{R}_1^T\mathbf{R}_0^{-1}\mathbf{u}$
2. $\mathbf{g} = \mathbf{T}^{-1}\mathbf{f}$
3. $\mathbf{h} = (\lambda\mathbf{K} - \mathbf{I})\mathbf{g}$
4. $\mathbf{p} = -(\frac{d\boldsymbol{S}}{d\lambda}\boldsymbol{z} + \frac{d\boldsymbol{s}}{d\lambda}) = \boldsymbol{\Psi}\mathbf{h} - \mathbf{t}$

Redefined factors

1. $a =< \mathbf{p}, \hat{\boldsymbol{\varepsilon}} >$

2.2 GCV-II-derivative

$\frac{d^2GCV}{d\lambda^2}(\lambda) = 2s\frac{d(dor^{-2}(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda})+<\boldsymbol{p},\hat{\boldsymbol{\varepsilon}}>))}{d\lambda}$

$[1] = \frac{d(dor^{-2})}{d\lambda}(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda})+ <\boldsymbol{p},\hat{\boldsymbol{\varepsilon}}>) = 2\frac{1}{dor^3}tr(\frac{d\boldsymbol{S}}{d\lambda})(\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda})+ <\boldsymbol{p},\hat{\boldsymbol{\varepsilon}}>)$

$[2] = \frac{1}{dor^2}\frac{d(\hat{\sigma}^2)}{d\lambda}tr(\frac{d\boldsymbol{S}}{d\lambda}) = \frac{1}{dor^2}\frac{\frac{d(SS_{res})}{d\lambda}dor - SS_{res}\frac{d(dor)}{d\lambda}}{dor^2}tr(\frac{d\boldsymbol{S}}{d\lambda}) = \frac{1}{dor^2}\frac{2<\boldsymbol{p},\hat{\boldsymbol{\varepsilon}}>dor + SS_{res}tr(\frac{d\boldsymbol{S}}{d\lambda})}{dor^2}tr(\frac{d\boldsymbol{S}}{d\lambda}) = \frac{1}{dor^3}(2<\boldsymbol{p},\hat{\boldsymbol{\varepsilon}}> + \hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}))tr(\frac{d\boldsymbol{S}}{d\lambda})$

$[3] = \frac{1}{dor^2}\hat{\sigma}^2 tr(\frac{d^2\boldsymbol{S}}{d\lambda^2})$

$[4] = \frac{1}{dor^2} <\frac{d\boldsymbol{p}}{d\lambda},\hat{\boldsymbol{\varepsilon}}> = \frac{1}{dor^2} < -\frac{d^2\boldsymbol{S}}{d\lambda^2}\boldsymbol{z} - \frac{d^2\boldsymbol{s}}{d\lambda^2},\hat{\boldsymbol{\varepsilon}}> = \frac{1}{dor^2} < -\frac{d^2\boldsymbol{S}}{d\lambda^2}\boldsymbol{z} - 2\boldsymbol{\Psi}\mathbf{Kh},\hat{\boldsymbol{\varepsilon}}>$

$[5] = \frac{1}{dor^2} <\boldsymbol{p},\frac{d\hat{\boldsymbol{\varepsilon}}}{d\lambda}> = \frac{1}{dor^2} <\boldsymbol{p},\boldsymbol{Q}\boldsymbol{p}>$

$\Longrightarrow \frac{d^2GCV}{d\lambda^2}(\lambda) =$
$= \frac{2s}{dor^2}\{\frac{1}{dor}[3\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}) + 4<\boldsymbol{p},\hat{\boldsymbol{\varepsilon}}>]tr(\frac{d\boldsymbol{S}}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2\boldsymbol{S}}{d\lambda^2}) + <\boldsymbol{p},\boldsymbol{Q}\boldsymbol{p}> + <\frac{d\boldsymbol{p}}{d\lambda},\hat{\boldsymbol{\varepsilon}}>\} =$
$= \frac{2s}{dor^2}\{\frac{1}{dor}[3\hat{\sigma}^2 tr(\frac{d\boldsymbol{S}}{d\lambda}) + 4a]tr(\frac{d\boldsymbol{S}}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2\boldsymbol{S}}{d\lambda^2}) + b + c\}$

Useful side computations

1. $\frac{d\boldsymbol{h}}{d\lambda} = -2\mathbf{Kh}$

Redefined factors

1. $b = <\boldsymbol{p},\boldsymbol{Q}\boldsymbol{p}>$
2. $c = <\frac{d\boldsymbol{p}}{d\lambda},\hat{\boldsymbol{\varepsilon}}>$

Chapter 3

Forcing term and nonhomogeneous Dirichlet

Define GCV_{homo} the computation of the GCV in the homogeneous case

3.1 GCV-I-derivative

$\frac{dGCV}{d\lambda}(\lambda) = \frac{d[GCV_{homo} + \frac{s}{dor^2}(||\mathbf{r}(\lambda)||^2 - 2 < \hat{\varepsilon}, \mathbf{r}(\lambda) >)]}{d\lambda} = \frac{dGCV_{homo}}{d\lambda} + s(||\mathbf{r}(\lambda)||^2 - 2 < \hat{\varepsilon}, \mathbf{r}(\lambda) >)\frac{d(dor^{-2})}{d\lambda} + \frac{2s}{dor^2}(< \mathbf{r}(\lambda), \frac{d\mathbf{r}}{d\lambda} > - < \frac{d\hat{\varepsilon}}{d\lambda}, \mathbf{r}(\lambda) > - < \hat{\varepsilon}, \frac{d\mathbf{r}(\lambda)}{d\lambda} >)$

$$V = \Psi^T \mathbf{A}\mathbf{Q}\Psi + \lambda \mathbf{R}_1^T \mathbf{R}_0^{-1} \mathbf{R}_1 \tag{3.1}$$

$$\frac{d\mathbf{V}^{-1}}{d\lambda} = -\mathbf{V}^{-1}\mathbf{R}_1^T \mathbf{R}_0^{-1} \mathbf{R}_1 \mathbf{V}^{-1} \tag{3.2}$$

$$\frac{d\mathbf{S}}{d\lambda} = -\Psi \frac{d\mathbf{V}^{-1}}{d\lambda} \Psi^T \mathbf{A}\mathbf{Q} \tag{3.3}$$

$$\frac{d\mathbf{r}}{d\lambda} = \frac{1}{\lambda}\mathbf{r}(\lambda) + \lambda \mathbf{Q}\Psi \frac{d\mathbf{V}^{-1}}{d\lambda} \mathbf{R}_1^T \mathbf{R}_0^{-1} \mathbf{u}^* \tag{3.4}$$

3.2 GCV-II-derivative

$$\begin{aligned}\frac{d^2GCV}{d\lambda^2} = & \frac{d^2GCV_{homo}}{d\lambda^2} + 2s(< \mathbf{r}(\lambda), \frac{d\mathbf{r}}{d\lambda} > - < \frac{d\hat{\varepsilon}}{d\lambda}, \mathbf{r}(\lambda) > - < \hat{\varepsilon}, \frac{d\mathbf{r}(\lambda)}{d\lambda} >)\frac{d(dor^{-2})}{d\lambda} + s(||\mathbf{r}(\lambda)||^2 \\ & - 2 < \hat{\varepsilon}, \mathbf{r}(\lambda) >)\frac{d^2}{d\lambda^2}(dor^{-2}) + 2\frac{s}{dor^2}[\ ||\frac{d\mathbf{r}}{d\lambda}||^2 + < \mathbf{r}, \frac{d^2\mathbf{r}}{d\lambda^2} > - < \frac{d^2\hat{\varepsilon}}{d\lambda}, \mathbf{r}(\lambda) > -2 < \frac{d\hat{\varepsilon}}{d\lambda}, \frac{d\mathbf{r}(\lambda)}{d\lambda} > \\ & - < \hat{\varepsilon}, \frac{d^2\mathbf{r}}{d\lambda^2} >] \\ & + 2s\frac{d(dor^{-2})}{d\lambda}[< \mathbf{r}(\lambda), \frac{d\mathbf{r}}{d\lambda} > - < \frac{d\hat{\varepsilon}}{d\lambda}, \mathbf{r}(\lambda) > - < \hat{\varepsilon}, \frac{d\mathbf{r}(\lambda)}{d\lambda} >]\end{aligned}$$

$$\frac{d^2\hat{\varepsilon}}{d\lambda^2} = -\mathbf{Q}\frac{d^2\mathbf{S}}{d\lambda^2}\mathbf{z} \tag{3.5}$$

$$\frac{d^2\mathbf{r}}{d\lambda^2} = -\frac{1}{\lambda^2}\mathbf{r}(\lambda) + \frac{1}{\lambda}\frac{d\mathbf{r}}{d\lambda} + \mathbf{Q}\Psi(\frac{d\mathbf{V}^{-1}}{d\lambda} + \lambda\frac{d^2\mathbf{V}^{-1}}{d\lambda^2})\mathbf{R}_1^T \mathbf{R}_0^{-1} \mathbf{u}^* \tag{3.6}$$

$$\frac{d^2\mathbf{V}^{-1}}{d\lambda^2} = -\frac{d\mathbf{V}^{-1}}{d\lambda}\mathbf{R}_1^T \mathbf{R}_0^{-1} \mathbf{R}_1 \mathbf{V}^{-1} - \mathbf{V}^{-1}\mathbf{R}_1^T \mathbf{R}_0^{-1} \mathbf{R}_1 \frac{d\mathbf{V}^{-1}}{d\lambda} \tag{3.7}$$

$$\frac{d\ dor}{d\lambda} = -tr(\frac{d\mathbf{S}(\lambda)}{d\lambda}) \tag{3.8}$$

$$\frac{d^2 dor^{-2}}{d\lambda^2} = 2tr(\frac{d^2\mathbf{S}(\lambda)}{d\lambda^2})dor^{-3} + 6\ dor^{-4}\{tr(\frac{d\mathbf{S}(\lambda)}{d\lambda})\}^2 \tag{3.9}$$