

Chapter 1

GCV

1.1 GCV-I-derivative

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

$$[1] = \frac{dSS_{res}}{d\lambda} = \frac{d(\langle \hat{\epsilon}, \hat{\epsilon} \rangle)}{d\lambda} = 2 \langle \frac{d\hat{\epsilon}}{d\lambda}, \hat{\epsilon} \rangle = 2 \langle \frac{d((Q-QS)z)}{d\lambda}, \hat{\epsilon} \rangle = -2 \langle Q \frac{dS}{d\lambda} z, \hat{\epsilon} \rangle \stackrel{Q \in Sym}{=} -2 \langle \frac{dS}{d\lambda} z, Q \hat{\epsilon} \rangle \stackrel{Q^2=Q}{=} -2 \langle \frac{dS}{d\lambda} z, \hat{\epsilon} \rangle$$

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

$$\implies \frac{dGCV}{d\lambda}(\lambda) = s(- \langle \frac{dS}{d\lambda} z, \hat{\epsilon} \rangle \frac{2}{dor^2} + SS_{res} \frac{2}{dor^3} tr(\frac{dS}{d\lambda})) = \frac{2s}{dor^2} (\hat{\sigma}^2 tr(\frac{dS}{d\lambda}) + a)$$

1.1.1 Fundamental matrices

1. $\mathbf{R} = \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1$
2. $\mathbf{T} = \Psi^t \mathbf{Q} \Psi + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1 = \Psi^t \mathbf{Q} \Psi + \lambda \mathbf{R}$
3. $\mathbf{V} = (\Psi^t \mathbf{Q} \Psi + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1)^{-1} \Psi^t \mathbf{Q} = \mathbf{T}^{-1} \Psi^t \mathbf{Q}$
4. $\mathbf{S} = \Psi (\Psi^t \mathbf{Q} \Psi + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1)^{-1} \Psi^t \mathbf{Q} = \Psi \mathbf{V}$
5. $\frac{dS}{d\lambda} = -\Psi (\Psi^t \mathbf{Q} \Psi + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1)^{-1} \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1 (\Psi^t \mathbf{Q} \Psi + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1)^{-1} \Psi^t \mathbf{Q}$
 $= -\Psi \mathbf{T}^{-1} \mathbf{R} \mathbf{V} = -\Psi \mathbf{K} \mathbf{V} = -\Psi \mathbf{F}$

Useful stored factors

1. $\mathbf{K} = \mathbf{T}^{-1} \mathbf{R}$
2. $\mathbf{F} = \mathbf{K} \mathbf{V}$
3. $\mathbf{t} = \frac{dS}{d\lambda} z$
4. $a = - \langle \frac{dS}{d\lambda} z, \hat{\epsilon} \rangle = - \langle \mathbf{t}, \hat{\epsilon} \rangle$

1.2 GCV-II-derivative

$$\frac{d^2 GCV}{d\lambda^2}(\lambda) = 2s \frac{d(dor^{-2}(\hat{\sigma}^2 tr(\frac{d\mathbf{S}}{d\lambda}) - \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \hat{\epsilon} \rangle))}{d\lambda}$$

$$[1] = \frac{d(dor^{-2})}{d\lambda} (\hat{\sigma}^2 tr(\frac{d\mathbf{S}}{d\lambda}) - \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \hat{\epsilon} \rangle) = 2 \frac{1}{dor^3} tr(\frac{d\mathbf{S}}{d\lambda}) (\hat{\sigma}^2 tr(\frac{d\mathbf{S}}{d\lambda}) - \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \hat{\epsilon} \rangle)$$

$$[2] = \frac{1}{dor^2} \frac{d(\hat{\sigma}^2)}{d\lambda} tr(\frac{d\mathbf{S}}{d\lambda}) = \frac{1}{dor^2} \frac{\frac{d(SS_{res})}{d\lambda} dor - SS_{res} \frac{d(dor)}{d\lambda}}{dor^2} tr(\frac{d\mathbf{S}}{d\lambda}) = \frac{1}{dor^2} \frac{-2 \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \hat{\epsilon} \rangle dor + SS_{res} tr(\frac{d\mathbf{S}}{d\lambda})}{dor^2} tr(\frac{d\mathbf{S}}{d\lambda}) = \frac{1}{dor^3} (-2 \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \hat{\epsilon} \rangle + \hat{\sigma}^2 tr(\frac{d\mathbf{S}}{d\lambda})) tr(\frac{d\mathbf{S}}{d\lambda})$$

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

$$[4] = -\frac{1}{dor^2} \langle \frac{d^2 \mathbf{S}}{d\lambda^2} \mathbf{z}, \hat{\epsilon} \rangle$$

$$[5] = -\frac{1}{dor^2} \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \frac{d\hat{\epsilon}}{d\lambda} \rangle = \frac{1}{dor^2} \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \mathbf{Q} \frac{d\mathbf{S}}{d\lambda} \mathbf{z} \rangle$$

$$\begin{aligned} \implies \frac{d^2 GCV}{d\lambda^2}(\lambda) &= \\ &= \frac{2s}{dor^2} \left\{ \frac{1}{dor} [3\hat{\sigma}^2 tr(\frac{d\mathbf{S}}{d\lambda}) - 4 \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \hat{\epsilon} \rangle] tr(\frac{d\mathbf{S}}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2 \mathbf{S}}{d\lambda^2}) + \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \mathbf{Q} \frac{d\mathbf{S}}{d\lambda} \mathbf{z} \rangle - \langle \frac{d^2 \mathbf{S}}{d\lambda^2} \mathbf{z}, \hat{\epsilon} \rangle \right\} = \\ &= \frac{2s}{dor^2} \left\{ \frac{1}{dor} [3\hat{\sigma}^2 tr(\frac{d\mathbf{S}}{d\lambda}) + 4a] tr(\frac{d\mathbf{S}}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2 \mathbf{S}}{d\lambda^2}) + b + c \right\} \end{aligned}$$

1.2.1 Fundamental matrices

$$\begin{aligned} 1. \quad \frac{d^2 \mathbf{S}}{d\lambda^2} &= 2\boldsymbol{\Psi}[(\boldsymbol{\Psi}^t \mathbf{Q} \boldsymbol{\Psi} + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1)^{-1} \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1]^2 (\boldsymbol{\Psi}^t \mathbf{Q} \boldsymbol{\Psi} + \lambda \mathbf{R}_1^t \mathbf{R}_0^{-1} \mathbf{R}_1)^{-1} \boldsymbol{\Psi}^t \mathbf{Q} \\ &= 2\boldsymbol{\Psi}(\mathbf{T}^{-1} \mathbf{R})^2 \mathbf{V} = 2\boldsymbol{\Psi} \mathbf{K}^2 \mathbf{V} = 2\boldsymbol{\Psi} \mathbf{K} \mathbf{F} \end{aligned}$$

Useful stored factors

1. $b = \langle \frac{d\mathbf{S}}{d\lambda} \mathbf{z}, \mathbf{Q} \frac{d\mathbf{S}}{d\lambda} \mathbf{z} \rangle = \langle \mathbf{t}, \mathbf{Q} \mathbf{t} \rangle$
2. $c = - \langle \frac{d^2 \mathbf{S}}{d\lambda^2} \mathbf{z}, \hat{\epsilon} \rangle$

Chapter 2

Forced GCV

2.1 GCV-I-derivative

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

$$[1] = \frac{dSS_{res}}{d\lambda} = \frac{d(<\hat{\epsilon}, \hat{\epsilon}>)}{d\lambda} = 2 < \frac{d\hat{\epsilon}}{d\lambda}, \hat{\epsilon} > = 2 < \frac{d((Q-QS)z-r)}{d\lambda}, \hat{\epsilon} > = -2 < Q(\frac{dS}{d\lambda}z + \frac{ds}{d\lambda}), \hat{\epsilon} > \stackrel{Q \in Sym}{=} \\ -2 < \frac{dS}{d\lambda}z + \frac{ds}{d\lambda}, Q\hat{\epsilon} > \stackrel{Q^2=Q}{=} 2 < \lambda h - (\frac{s}{\lambda} + t), \hat{\epsilon} > = 2a$$

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

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

Useful side computations

$$1. \frac{ds}{d\lambda} = \frac{s}{\lambda} - \lambda \Psi T^{-1} R T^{-1} R_1^T R_0^{-1} u = \frac{s}{\lambda} - \lambda \Psi K g = \frac{s}{\lambda} - \lambda \Psi k = \frac{s}{\lambda} - \lambda h$$

Useful stored factors

1. $f = R_1^T R_0^{-1} u$
2. $g = T^{-1} f$
3. $k = K g$
4. $h = \Psi k$
5. $s = \lambda \Psi T^{-1} R_1^T R_0^{-1} u = \lambda \Psi g$
6. $r = \lambda Q \Psi T^{-1} R_1^T R_0^{-1} u = \lambda Q \Psi g = Q s$
7. $p = \lambda h - (\frac{s}{\lambda} + t)$

Redefined factors

1. $a = < p, \hat{\epsilon} >$

2.2 GCV-II-derivative

$$\frac{d^2 GCV}{d\lambda^2}(\lambda) = 2s \frac{d(dor^{-2}(\hat{\sigma}^2 tr(\frac{dS}{d\lambda}) + \langle \mathbf{p}, \hat{\epsilon} \rangle))}{d\lambda}$$

$$[1] = \frac{d(dor^{-2})}{d\lambda}(\hat{\sigma}^2 tr(\frac{dS}{d\lambda}) + \langle \mathbf{p}, \hat{\epsilon} \rangle) = 2 \frac{1}{dor^3} tr(\frac{dS}{d\lambda})(\hat{\sigma}^2 tr(\frac{dS}{d\lambda}) + \langle \mathbf{p}, \hat{\epsilon} \rangle)$$

$$[2] = \frac{1}{dor^2} \frac{d(\hat{\sigma}^2)}{d\lambda} tr(\frac{dS}{d\lambda}) = \frac{1}{dor^2} \frac{\frac{d(SS_{res})}{d\lambda} dor - SS_{res} \frac{d(dor)}{d\lambda}}{dor^2} tr(\frac{dS}{d\lambda}) = \frac{1}{dor^2} \frac{\langle \mathbf{p}, \hat{\epsilon} \rangle dor + SS_{res} tr(\frac{dS}{d\lambda})}{dor^2} tr(\frac{dS}{d\lambda}) = \frac{1}{dor^3} (2 \langle \mathbf{p}, \hat{\epsilon} \rangle + \hat{\sigma}^2 tr(\frac{dS}{d\lambda})) tr(\frac{dS}{d\lambda})$$

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

$$[4] = \frac{1}{dor^2} \langle \frac{d\mathbf{p}}{d\lambda}, \hat{\epsilon} \rangle = \frac{1}{dor^2} \langle -\frac{d^2 \mathbf{S}}{d\lambda^2} \mathbf{z} + \frac{\mathbf{s}}{\lambda^2} + \mathbf{h} + \lambda \frac{d\mathbf{h}}{d\lambda} - \frac{1}{\lambda} \frac{d\mathbf{s}}{d\lambda}, \hat{\epsilon} \rangle = \frac{1}{dor^2} \langle -\frac{d^2 \mathbf{S}}{d\lambda^2} \mathbf{z} + \frac{\mathbf{s}}{\lambda^2} + \mathbf{h} - 2\lambda \Psi \mathbf{K} \mathbf{k} - \frac{\mathbf{s}}{\lambda^2} + \mathbf{h}, \hat{\epsilon} \rangle = \frac{1}{dor^2} \langle -\frac{d^2 \mathbf{S}}{d\lambda^2} \mathbf{z} + 2\mathbf{h} - 2\lambda \Psi \mathbf{K} \mathbf{k}, \hat{\epsilon} \rangle$$

$$[5] = \frac{1}{dor^2} \langle \mathbf{p}, \frac{d\hat{\epsilon}}{d\lambda} \rangle = \frac{1}{dor^2} \langle \mathbf{p}, \mathbf{Qp} \rangle$$

$$\begin{aligned} \implies \frac{d^2 GCV}{d\lambda^2}(\lambda) &= \\ &= \frac{2s}{dor^2} \left\{ \frac{1}{dor} [3\hat{\sigma}^2 tr(\frac{dS}{d\lambda}) + 4 \langle \mathbf{p}, \hat{\epsilon} \rangle] tr(\frac{dS}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2 S}{d\lambda^2}) + \langle \mathbf{p}, \mathbf{Qp} \rangle + \langle \frac{d\mathbf{p}}{d\lambda}, \hat{\epsilon} \rangle \right\} = \\ &= \frac{2s}{dor^2} \left\{ \frac{1}{dor} [3\hat{\sigma}^2 tr(\frac{dS}{d\lambda}) + 4a] tr(\frac{dS}{d\lambda}) + \hat{\sigma}^2 tr(\frac{d^2 S}{d\lambda^2}) + b + c \right\} \end{aligned}$$

Useful side computations

$$1. \frac{d\mathbf{h}}{d\lambda} = -2\Psi \mathbf{T}^{-1} \mathbf{R} \mathbf{T}^{-1} \mathbf{R} \mathbf{T}^{-1} \mathbf{f} = -2\Psi \mathbf{K} \mathbf{k}$$

Redefined factors

1. $b = \langle \mathbf{p}, \mathbf{Qp} \rangle$
2. $c = \langle \frac{d\mathbf{p}}{d\lambda}, \hat{\epsilon} \rangle$

Chapter 3

Forcing term and nonhomogeneous Dirichlet

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

3.1 GCV-I-derivative

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

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

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

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

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

3.2 GCV-II-derivative

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

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

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

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

$$\frac{d \, dor}{d\lambda} = -tr\left(\frac{d\mathbf{S}(\lambda)}{d\lambda}\right) \quad (3.8)$$

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