

Gaussian Process object which handles Angles

Rowan McAllister

June 26, 2015

Titsias method: “Variational Learning of Inducing Variables in Sparse Gaussian Processes”

Using Eq.9 from Titsias paper, plus extra terms V , C and U :

$$\begin{aligned}
 \text{nllml} &\triangleq -\log[\mathcal{N}(\mathbf{y}; 0, \sigma^2 \mathbf{I}_n + \mathbf{Q}_{nn})] + \frac{1}{2\sigma^2} \text{Tr}(\mathbf{K}_{nn} - \mathbf{Q}_{nn}) \\
 &= \frac{1}{2} (n \log[2\pi] + \log[\det[\sigma^2 \mathbf{I}_n + \mathbf{Q}_{nn}]] + \mathbf{y}^\top (\sigma^2 \mathbf{I}_n + \mathbf{Q}_{nn})^{-1} \mathbf{y} + \sigma^{-2} \text{Tr}(\mathbf{K}_{nn} - \mathbf{Q}_{nn})) \\
 \mathbf{Q}_{nn} &\triangleq \mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn} \\
 &= \mathbf{V}^\top \mathbf{V} \\
 \mathbf{V} &= \mathbf{L}^{-\top} \mathbf{K}_{mn} = \text{chol}(\mathbf{K}_{mm})^\top \setminus \mathbf{K}_{mn} \\
 \mathbf{K}_{mm} &= \mathbf{L}^\top \mathbf{L} \\
 \mathbf{C} &\triangleq \text{chol}(\sigma^2 \mathbf{I}_m + \mathbf{V} \mathbf{V}^\top) \\
 \mathbf{U} &\triangleq (\sigma^2 \mathbf{I}_m + \mathbf{V} \mathbf{V}^\top)^{-\frac{\top}{2}} = \mathbf{C}^\top \setminus \mathbf{V}
 \end{aligned} \tag{1}$$

Using matrix inversion lemma:

$$\begin{aligned}
 (\sigma^2 \mathbf{I}_n + \mathbf{Q}_{nn})^{-1} &= (\sigma^2 \mathbf{I}_n + \mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn})^{-1} \\
 &= \sigma^{-2} \mathbf{I}_n - \sigma^{-2} \mathbf{K}_{nm} (\mathbf{K}_{mm} + \sigma^{-2} \mathbf{K}_{mn} \mathbf{K}_{nm})^{-1} \mathbf{K}_{mn} \sigma^{-2} \\
 &= \sigma^{-2} (\mathbf{I}_n - \mathbf{K}_{nm} \underbrace{(\sigma^2 \mathbf{L}^\top \mathbf{L} + \mathbf{K}_{mn} \mathbf{K}_{nm})^{-1}}_{\mathbf{A}} \mathbf{K}_{mn}) \\
 &= \sigma^{-2} (\mathbf{I}_n - \mathbf{K}_{nm} \mathbf{L}^{-1} (\sigma^2 \mathbf{I}_m + \mathbf{L}^{-\top} \mathbf{K}_{mn} \mathbf{K}_{nm} \mathbf{L}^{-1})^{-1} \mathbf{L}^{-\top} \mathbf{K}_{mn}) \\
 &= \sigma^{-2} (\mathbf{I}_n - \mathbf{V}^\top (\sigma^2 \mathbf{I}_m + \mathbf{V} \mathbf{V}^\top)^{-1} \mathbf{V}) \\
 &= \sigma^{-2} (\mathbf{I}_n - \mathbf{U}^\top \mathbf{U})
 \end{aligned} \tag{2}$$

For the determinant we make use of identity:

$$\det(\mathbf{a} \mathbf{I}_n \pm \mathbf{C} \mathbf{A}^{-1} \mathbf{B}) = \mathbf{a}^{n-m} \det(\mathbf{a} \mathbf{A} \pm \mathbf{B} \mathbf{C}) / \det(\mathbf{A}) \quad \text{where } \mathbf{A} \in \mathbb{R}^{m \times m}, \mathbf{B} \in \mathbb{R}^{m \times n}, \mathbf{C} \in \mathbb{R}^{n \times m}, \mathbf{a} \in \mathbb{R} \tag{3}$$

and thus have:

$$\begin{aligned}
 \det[\sigma^2 \mathbf{I} + \mathbf{Q}_{nn}] &= \det[\sigma^2 \mathbf{I} + \mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn}] \\
 &= \sigma^{2(n-m)} \det[\sigma^2 \mathbf{K}_{mm} + \mathbf{K}_{mn} \mathbf{K}_{nm}] / \det[\mathbf{K}_{mm}] \\
 &= \sigma^{2(n-m)} \det[\sigma^2 \mathbf{I}_m + \mathbf{V} \mathbf{V}^\top] \\
 &= \sigma^{2(n-m)} (\prod \text{diag}(\mathbf{C}))^2 \\
 \log[\det[\sigma^2 \mathbf{I} + \mathbf{Q}_{nn}]] &= (n-m) \log[\sigma^2] + 2 \sum \log[\text{diag}(\mathbf{C})]
 \end{aligned} \tag{4}$$

For the trace:

$$\begin{aligned}\text{Tr}(\mathbf{K}_{nn} - \mathbf{Q}_{nn}) &= \text{Tr}(\mathbf{K}_{nn}) - \text{Tr}(\mathbf{V}^\top \mathbf{V}) \\ &= n\sigma_{\text{signal}}^2 - \sum_{ij} (\mathbf{V} \odot \mathbf{V})_{ij}\end{aligned}\quad (5)$$

Derivatives

We use derivatives tricks from Ed Snelson's PhD thesis "Flexible and efficient Gaussian process models for machine learning", appendix C:

$$\begin{aligned}\mathbf{Q}_{nn} &\triangleq \mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn} \\ \mathbf{q}_{nn} &\triangleq \sigma^2 \mathbf{I}_n + \mathbf{Q}_{nn} \\ \mathbf{A} &= \sigma^2 \mathbf{K}_{mm} + \mathbf{K}_{mn} \mathbf{K}_{nm} \\ \dot{\mathbf{A}} &= \sigma^2 \dot{\mathbf{K}}_{mm} + \dot{\mathbf{K}}_{mn} \mathbf{K}_{nm} + \mathbf{K}_{mn} \dot{\mathbf{K}}_{nm} \\ \mathbf{B} &= \mathbf{K}_{mn}^\top \mathbf{A}^{-1} \\ \frac{\partial}{\partial \mathbf{x}_{mf}} n \ln l &= \frac{1}{2} \left(\underbrace{\frac{\partial}{\partial \mathbf{x}_{mf}} \log[\det[\mathbf{q}_{nn}]]}_{\mathcal{L}_1} + \underbrace{\frac{\partial}{\partial \mathbf{x}_{mf}} \mathbf{y}^\top \mathbf{q}_{nn}^{-1} \mathbf{y}}_{\mathcal{L}_2} + \sigma^{-2} \underbrace{\frac{\partial}{\partial \mathbf{x}_{mf}} \text{Tr}(-\mathbf{Q}_{nn})}_{\mathcal{L}_3} \right)\end{aligned}\quad (6)$$

$$\begin{aligned}\mathcal{L}_1 &= \log[\det[\mathbf{q}_{nn}]] \\ &= \log[\det[\mathbf{A}]] - \log[\det[\mathbf{K}_{mm}]] + (N - M) \log \sigma^2 \\ \dot{\mathcal{L}}_1 &= \text{Tr}(\mathbf{A}^{-\frac{\top}{2}} \dot{\mathbf{A}} \mathbf{A}^{-\frac{1}{2}}) - \text{Tr}(\mathbf{K}_{mm}^{-\frac{\top}{2}} \dot{\mathbf{K}}_{mm} \mathbf{K}_{mm}^{-\frac{1}{2}}) \quad (\text{see Eq C.8 Ed's thesis})\end{aligned}$$

$$\begin{aligned}\mathcal{L}_2 &= \mathbf{y}^\top \mathbf{q}_{nn}^{-1} \mathbf{y} \\ \dot{\mathcal{L}}_2 &= \frac{1}{\sigma^2} \mathbf{y}^\top [\mathbf{K}_{mn}^\top \mathbf{A}^{-\frac{1}{2}} (\mathbf{A}^{-\frac{\top}{2}} \dot{\mathbf{A}} \mathbf{A}^{-\frac{1}{2}} (\mathbf{A}^{-\frac{\top}{2}} \mathbf{K}_{mn}) - 2 \mathbf{A}^{-\frac{\top}{2}} \dot{\mathbf{K}}_{mn})] \mathbf{y} \quad (\text{see Eq C.9 Ed's thesis}) \\ &= \frac{1}{\sigma^2} \mathbf{y}^\top [\mathbf{B} (\dot{\mathbf{A}} \mathbf{B}^\top - 2 \dot{\mathbf{K}}_{mn})] \mathbf{y}\end{aligned}\quad (7)$$

$$\begin{aligned}\mathcal{L}_3 &= \text{Tr}(-\mathbf{Q}_{nn}) \\ &= -\text{Tr}(\mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn}) \\ \dot{\mathcal{L}}_3 &= -\text{Tr}(\dot{\mathbf{Q}}_{nn}) \\ &= -\text{Tr}(-\mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \dot{\mathbf{K}}_{mm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn} + \dot{\mathbf{K}}_{nm} \mathbf{K}_{mm}^{-1} \mathbf{K}_{mn} + \mathbf{K}_{nm} \mathbf{K}_{mm}^{-1} \dot{\mathbf{K}}_{mn});\end{aligned}$$