x

θ_*

$f_{\theta_*}(-)$

$$P(y|x) = \mathcal{N}(f_{\theta_*}(x), J(x) * \Sigma * J(x)^T)$$

Σ

$J(x)$

$f_\theta(x)$

θ

f_θ

$$A(x)$$

$$A(x) * A(x)^T \approx J(x) * \Sigma * J(x)^T$$

$$f(x, \theta)$$

$$f : X \times \Theta \to Y$$

X

Θ

Y

$$X \simeq \mathbb{R}^n$$

$$\Theta \simeq \mathbb{R}^w$$

$$Y \simeq \mathbb{R}^d$$

$$(x, \theta) \mapsto f(x, \theta)$$

f

$$\theta = \theta_*$$

$$f_{\theta_*} : X \to Y$$

$$f_{\theta_*}(x) = f(x, \theta_*)$$

$$P(\theta|D)$$

$$\theta_{\mathrm{MAP}} = \operatorname{argmin}_{\theta \in W} \log P(D|\theta) + \log P(\theta)$$

$$D := (x_n, y_n) \in X \times Y_{n=1}^{N}$$

$\theta \in \Theta$

$$\mathcal{L}(D;\theta) = \log P(D|\theta) + \log P(\theta)$$

$$P(y|x)$$

$$f(x, -) : \Theta \to Y$$

$$P(y|x) = f(x, -)_* P(\theta|D)$$

$$\hat{f}(x)$$

$$\hat{f}(x) = \mathbb{E}_{y \sim P(y|x)}[y] = \mathbb{E}_{\theta \sim P(\theta|D)}\left[f(x, \theta)\right]$$

$(\hat{f}(x)) =$

$_{y\sim P(y|x)}[y] =$

$$\theta \sim P(\theta|D) \, [f(x, \theta)]$$

$$\theta_1, \cdots, \theta_k \sim P(\theta|D)$$

$$\{f(x,\theta_i)\}_{i=1}^{k} \sim P(y|x)$$

$$\overline{\hat{f}(x)} = \frac{1}{k}\sum_{i=1}^{k} f(x,\theta_i) \in \mathbb{R}^d$$

$$\overline{\operatorname{unc}(\hat{f}(x))} = \frac{1}{k-1} \sum_{i=1}^{k} f(x, \theta_i) f(x, \theta_i)^T \in \mathbb{R}^{d \times d}$$

$$\overline{\mathrm{unc}(\hat{f}(x))}$$

$$\overline{\hat{f}(x)}$$

$$f(x, \theta_{\mathrm{MAP}})$$

$$\theta_{\text{MAP}}$$

$$P(\theta|D) \sim_{LA} \mathcal{N}(\theta_{\mathrm{MAP}}, \Sigma)$$

$$\Sigma \in \mathbb{R}^{w \times w}$$

$$\Sigma := \left(\frac{\partial^2}{\partial \theta^2} \mathcal{L}(D; \theta) \Big|_{\theta_{\mathrm{MAP}}} \right)^{-1}$$

$$I_\theta(\theta_{\mathrm{MAP}}) = \mathrm{Cov}_{(x,y)\sim D}\left(\frac{\partial}{\partial\theta}\mathcal{L}((x,y);\theta)\bigg|_{\theta_{\mathrm{MAP}}}\right)$$

$$\boxed{\Sigma \sim I_\theta(\theta_{\mathrm{MAP}})^{-1}}$$

$$\theta = \theta_{\mathrm{MAP}}$$

$$f_{\mathrm{lin}}(x,\theta) = f(x,\theta_{\mathrm{MAP}}) + \left[\frac{\partial}{\partial\theta} f(x,\theta)\Big|_{\theta_{\mathrm{MAP}}} \right] (\theta - \theta_{\mathrm{MAP}})$$

$$\frac{\partial}{\partial\theta} f(x,\theta)\Big|_{\theta_{\mathrm{MAP}}}$$

$J(x) \in \mathbb{R}^{d \times w}$

$$\mathcal{N}(\theta_{\mathrm{MAP}}, \Sigma)$$

$$P_{\text{lin}}(y|x)$$

$$N(\theta_{\mathrm{MAP}}, \Sigma)$$

$$f_{\mathrm{lin}}(x,-) : \Theta \to Y$$

$$f_{\text{lin}}(x, \theta)$$

$$\mathbb{E}_{y \sim P_{\text{lin}}(y|x)}[y]$$

$$= \mathbb{E}_{\theta \sim \mathcal{N}(\theta_{\mathrm{MAP}}, \Sigma)} \left[f_{\mathrm{lin}}(x, \theta) \right]$$

$$= f(x, \theta_{\mathrm{MAP}}) + J(x) * \mathbb{E}_{\theta \sim \mathcal{N}(\theta_{\mathrm{MAP}}, \Sigma)} \left[(\theta - \theta_{\mathrm{MAP}}) \right]$$

$$= f(x, \theta_{\text{MAP}})$$

$$\mathbb{E}_{y \sim P_{\text{lin}}(y|x)}[y]$$

$=$

$$\theta \sim \mathcal{N}(\theta_{\mathrm{MAP}}, \Sigma) \left[f_{\mathrm{lin}}(x, \theta) \right]$$

$$\theta \sim \mathcal{N}(\theta_{\mathrm{MAP}}, \Sigma) \left[J(x) * (\theta - \theta_{\mathrm{MAP}}) \right]$$

$$\underset{\eta \sim \mathcal{N}(0,\Sigma)}{} [J(x) * \eta]$$

$$= J(x) * \Sigma * J(x)^T$$

$$\hat{f}_{\mathrm{lin}}(x)$$

$$\hat{f}_{\mathrm{lin}}(x) = f(x, \theta_{\mathrm{MAP}})$$

$$\boxed{\mathrm{unc}(\hat{f}_{\mathrm{lin}}(x)) = J(x) * \Sigma * J(x)^T}$$

$$I = I_\theta(\theta_{\mathrm{MAP}})$$

$w \times w$

I

$$I \in \mathbb{R}^{w \times w}$$

$I_{(l)} \in \mathbb{R}^{w_l \times w_l},$

w_l

l

$\sum_{l=1}^{L} w_l = w$

$$w^2$$

$$\sum w_l^2$$

∇_l

$$\nabla_l = a_{l-1} \otimes g_l$$

a_{l-1}

$$l - 1$$

g_l

$$I_{(l)} = \mathbb{E}\left[\nabla_l * \nabla_l^T\right] = \mathbb{E}\left[(a_{l-1} \otimes g_l) * (a_{l-1} \otimes g_l)^T\right]$$

$$I_{(l)} \approx \mathbb{E}\left[a_{l-1} \otimes a_{l-1}^T\right] \otimes \mathbb{E}\left[g_l \otimes g_l^T\right] =: Q_{(l)} \otimes H_{(l)}$$

$$Q_{(l)} \in \mathbb{R}^{l_{\text{in}} \times l_{\text{in}}}$$

$$H_{(l)} \in \mathbb{R}^{l_{\text{out}} \times l_{\text{out}}}$$

$\mathbb{R}^{l_{\text{in}}} \to \mathbb{R}^{l_{\text{out}}}$

$$\sum w_l^2 = \sum (l_{\text{in}} l_{\text{out}})^2$$

$$\sum(l_{\text{in}}^2 + l_{\text{out}}^2)$$

$$I_{\mathrm{KFAC}} = \mathrm{diag}\left[Q_{(1)} \otimes H_{(1)}, \cdots, Q_{(L)} \otimes H_{(L)}\right]$$

Σ_{KFAC}

$$\begin{pmatrix} Q_{(1)}^{-1} \otimes H_{(1)}^{-1} & & \\ & \ddots & \\ & & Q_{(L)}^{-1} \otimes H_{(L)}^{-1} \end{pmatrix}$$

$$I_\theta(\theta_{\mathrm{MAP}})$$

$\theta_1, \ldots, \theta_w$

$$\frac{\partial f_i}{\partial \theta_j}$$

$$\frac{\partial}{\partial \theta_j} f_i(x, \theta) \bigg|_{\theta=\theta_{\mathrm{MAP}}}$$

$(f_1, \ldots, f_d)$

$f_i, 1 \leq i \leq d$

$$J(x) = \begin{pmatrix} - & [\nabla f_1]^T & - \\ & \vdots & \\ - & [\nabla f_d]^T & - \end{pmatrix}$$

d

$$(\hat{f}_{\text{lin}}(x)) = J(x)_{\text{KF}} * \Sigma_{\text{KFAC}} * J(x)_{\text{KF}}^T$$

$$J(x)_{\mathrm{KF}}$$

$d = 1$

$$f(x, \theta) \to \mathbb{R}$$

$$\frac{\partial}{\partial \theta} f(x, \theta) \Big|_{\theta_{\mathrm{MAP}}} \in \mathbb{R}^{1 \times w}$$

$l \in [1, \cdots, L]$

$$\frac{\partial}{\partial \theta_l} f(x, \theta)\bigg|_{\theta_{\mathrm{MAP}}} = a_{l-1} \otimes g_l$$

$$a_{l-1} \in \mathbb{R}^{1 \times l_{\text{in}}}$$

$g_l \in \mathbb{R}^{1 \times l_{\text{out}}}$

$J(x)$

$$= \left(\frac{\partial}{\partial \theta_1} f(x,\theta)\bigg|_{\theta_{\mathrm{MAP}}}, \cdots, \frac{\partial}{\partial \theta_L} f(x,\theta)\bigg|_{\theta_{\mathrm{MAP}}} \right)$$

$\in \mathbb{R}^{d\times(w_1+\cdots+w_L)}$

$$= \begin{pmatrix} | & & | \\ a_0^j \otimes g_1^j & \cdots & a_{L-1}^j \otimes g_L^j \\ | & & | \end{pmatrix}$$

$j \in (1, \cdots, d)$

$$J(x) * \begin{pmatrix} Q_{(1)}^{-1} \otimes H_{(1)}^{-1} & & \\ & \ddots & \\ & & Q_{(L)}^{-1} \otimes H_{(L)}^{-1} \end{pmatrix} * J(x)^T$$

$$_{j=1}^{d} \left[\sum_{l=1}^{L} \left(a_{l-1}^{j} * Q_{(l)}^{-1} * {a_{l-1}^{j}}^{T} \right) \otimes \left(g_{l}^{j} * H_{(l)}^{-1} * {g_{l-1}^{j}}^{T} \right) \right]$$

$$J(x) * \Sigma * J(x)^T$$

$$\eta \in \mathcal{N}(0, \Sigma) \left[J(x) * \eta \right]$$

$$\approx \frac{1}{N-1} \sum_{i=1}^{N} \left[J(x) * \eta_i\right] \left[J(x) * \eta_i\right]^T$$

$$(\eta_1, \cdots, \eta_n) \sim \mathcal{N}(0, \Sigma)$$

η

$$T_{\theta_{\mathrm{MAP}}}(\Theta)$$

$$J(x) * \eta$$

$$D_{\vec{\eta}} f = \lim_{h \to 0} \left(f(\theta_{\mathrm{MAP}} + h\vec{\eta}) - f(\theta_{\mathrm{MAP}}) \right) / h$$

$$(\vec{\eta}_1, \ldots, \vec{\eta}_k) \sim \mathcal{N}(0, \Sigma)^{\times k}$$

$$k \ll w$$

$$\overline{A}(x) := \begin{pmatrix} | & & | \\ \bar{D}_{\vec{\eta}_1} f & \cdots & \bar{D}_{\vec{\eta}_k} f \\ | & & | \end{pmatrix} \in \mathbb{R}^{d \times k}$$

$\bar{D}$

$$(f(x, \theta_{\mathrm{MAP}})) := \overline{A}(x) * \overline{A}(x)^T$$

$$\Sigma = B * B^T$$

$$J(x) * \Sigma * J(x)^T$$

$$A(x) * A(x)^T$$

$$A(x) = J(x) * B$$

B

$T_{\theta_{\mathrm{MAP}}}(W)$

n

$$\vec{z} \sim \mathcal{N}(\vec{\mu}, \Sigma)$$

$$\vec{z} = \vec{\mu} + B\vec{x}$$

$n \times n$

$$BB^T = \Sigma$$

$$\vec{x} \sim \mathcal{N}(\vec{0}, I_n)$$

$B =$

$$(\Sigma)$$

$$(Q_{(l)})^{-1} \otimes$$

$$(H_{(l)})^{-1}$$

$$\mathcal{N}(\vec{\mu}_l, Q_{(l)}^{-1} \otimes H_{(l)}^{-1})$$

$$\mathcal{N}(\vec{\mu}, \Sigma_{\text{KFAC}})$$

f_{θ_l}

$\vec{z}_l$

$$= \left(\mathrm{ch}(Q_{(l)})^{-1} \otimes \mathrm{ch}(H_{(l)})^{-1}\right) * \vec{x}_l$$

$$(Q_{(l)})^{-1} * \vec{x}_l$$

$$(l_{\mathrm{in}}, l_{\mathrm{out}}) * \mathrm{ch}(H_{(l)})^{-1}$$

$$\vec{x}_l \sim \mathcal{N}(\vec{\mu}_l, I_{w_l})$$