Multiclass logistic regression { Lecture 9

Now consider $K > 2$:

$$p(C_k|\vec{\varphi}) \equiv y_k(\vec{\varphi}) = \frac{e^{a_k}}{\sum_{j=1}^{K} e^{a_j}}$$

$$a_k = \vec{w}_k^T \cdot \vec{\varphi}$$

The goal is to determine $\{\vec{w}_k\}$ directly.

Use $\vec{t}_n = \{ t_{n,1} \dots \underbrace{t_{n,k}}_{\text{"1 if } \vec{t}_n \in C_k\text{, all other entries } = 0} \dots t_{n,K} \}$

$$T = \left(\overbrace{\qquad\qquad}^{K} \right\} N \qquad T_{nk} = t_{nk}$$

Then

$$\mathcal{L} = p(T | \vec{w}_1 \dots \vec{w}_K) = \prod_{n=1}^{N} \prod_{k=1}^{K} \underbrace{p(C_k | \overbrace{\vec{\varphi}_n}^{\vec{\varphi}(\vec{x}_n)})}_{y_{nk}}^{t_{nk}} \quad (=)$$

$$(=) \prod_{n=1}^{N} \prod_{k=1}^{K} y_{nk}^{t_{nk}}$$

$$E(\vec{w}_1, \dots, \vec{w}_K) = -\log \mathcal{L} = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \log y_{nk}.$$

Now, consider

$$\frac{\partial E}{\partial \vec{w}_j} = -\sum_n \sum_k t_{nk} \frac{1}{y_{nk}} \underbrace{\frac{\partial y_{nk}}{\partial \vec{w}_j}}_{\text{"} \frac{\partial y_{nk}}{\partial a_j} \frac{\partial a_j}{\partial \vec{w}_j}} \quad (=)$$

$\frac{\partial E}{\partial \vec{w}_j}$: vector derivative

$\frac{\partial a_j}{\partial \vec{w}_j} = \vec{\varphi}_n$

note that $\frac{\partial a_{j'}}{\partial \vec{w}_j} = 0, \; j' \neq j$

$$\frac{\partial y_k}{\partial a_j} = y_k \delta_{kj} - \frac{e^{a_k}}{\left(\sum_{j'} e^{a_{j'}}\right)^2} e^{a_j} =$$

$$= y_k \delta_{kj} - y_k y_j .$$

$$\boxed{=} - \sum_{n,k} \frac{t_{nk}}{y_{nk}} \left[y_{nk} \delta_{kj} - y_{nk} y_{nj} \right] \vec{y}_n =$$

$$= \sum_{n,k} \left[t_{nk} y_{nj} - t_{nk} \delta_{kj} \right] \vec{y}_n = \sum_n \left[y_{nj} - t_{nj} \right] \vec{y}_n .$$

$$\uparrow \quad \sum_k t_{nk} = 1 \quad , \forall n .$$

Moreover, $H = \underbrace{\frac{\partial^2 E}{\partial \vec{w}_k \partial \vec{w}_j}}_{MK \times MK \text{ matrix}} = \sum_n \left[\frac{\partial y_{nj}}{\partial \vec{w}_k} \right] \vec{y}_n =$

$$= \sum_n \left[y_{nj} \delta_{kj} - y_{nk} y_{nj} \right] \underbrace{\vec{y}_n \vec{y}_n^T}_{M \times M \text{ matrix}}$$

Can show that $\underbrace{\vec{u}^T H \vec{u} > 0}_{\text{positive definite}} \Rightarrow$ unique minimum

Thus can do NR algorithm again.

Probit regression

If desired, $\sigma(a)$ can be replaced by

$$\Phi(a) = \int_{-\infty}^{a} d\theta \, \mathcal{N}(\theta|0,1)$$ ← cumulative gaussian, or probit function

Indeed, consider $\sigma(a) = \frac{1}{1+e^{-a}}$ vs. $\Phi(\lambda a)$.

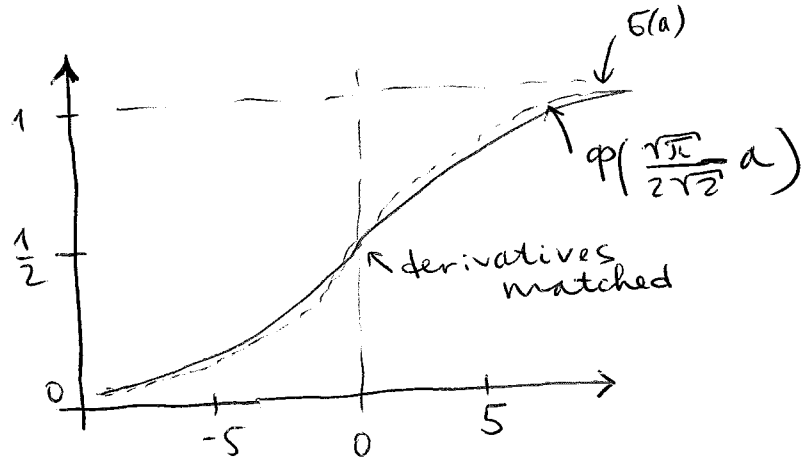
$$\left.\frac{d\sigma(a)}{da}\right|_{a=0} = \sigma(0)(1-\sigma(0)) = \frac{1}{4}.$$

But $$\left.\frac{d\Phi(\lambda a)}{da}\right|_{a=0} = \left.\frac{d\Phi(\lambda a)}{d(\lambda a)}\lambda\right|_{a=0} = \left.\frac{\lambda}{\sqrt{2\pi}} e^{-(\lambda a)^2}\right|_{a=0} = \frac{\lambda}{\sqrt{2\pi}}.$$

Match derivatives at $a=0$:

$$\frac{\lambda}{\sqrt{2\pi}} = \frac{1}{4} \Rightarrow \lambda^2 = \frac{\pi}{8}.$$

So, $\sigma(a) \approx \Phi\left(\frac{\sqrt{\pi}}{2\sqrt{2}} a\right)$:



Can repeat the ML analysis for the logistic regression with probit regression ⇒ similar results in practice.

Laplace approximation
(saddle-point appr'n)

Consider

$$p(z) = \frac{f(z)}{Z}$$

$$\int dz\, p(z) = 1 \Rightarrow Z = \int dz\, f(z).$$

$$f(z) \simeq f(z_0)\, e^{-\frac{A}{2}(z-z_0)^2}$$

$$A = -\frac{d^2}{dz^2} \log f(z)\Big|_{z_0}$$

$$\frac{df(z)}{dz}\Big|_{z_0} = 0 \quad \text{@ max}$$

$$\Rightarrow \frac{d \log f(z)}{dz}\Big|_{z_0} = 0 \text{ as well}$$

$$\log f(z) \simeq \log f(z_0) - \frac{1}{2} A (z-z_0)^2$$

Then $p(z) \Rightarrow q(z) = \sqrt{\frac{A}{2\pi}}\, e^{-\frac{A}{2}(z-z_0)^2} = \mathcal{N}(z \mid z_0, A^{-1})$

Likewise, $\vec{z}_0$ ← stationary point

$$f(\vec{z}) \simeq f(\vec{z}_0)\, e^{-\frac{1}{2}(\vec{z}-\vec{z}_0)^T A (\vec{z}-\vec{z}_0)}$$

$$p(\vec{z}) \Rightarrow q(\vec{z}) = \frac{|A|^{1/2}}{(2\pi)^{D/2}}\, e^{-\frac{1}{2}(\vec{z}-z_0)^T A (\vec{z}-\vec{z}_0)} =$$

$$= \mathcal{N}(\vec{z} \mid \vec{z}_0, A^{-1})$$

$$A = -\vec{\nabla}_{\vec{z}}\, \vec{\nabla}_{\vec{z}} \log f(\vec{z})\Big|_{\vec{z}_0}$$

$D \times D$ matrix

Note that

$$Z = \underbrace{\int d\vec{z}\, f(\vec{z})}_{\sim f(\vec{z}_0) \int e^{-\frac{1}{2}(\vec{z}-\vec{z}_0)^T A (\vec{z}-\vec{z}_0)} d\vec{z}} \simeq \underbrace{f(\vec{z}_0)\, \frac{(2\pi)^{D/2}}{|A|^{1/2}}}_{\text{saddle-point approx'n}}$$

Model comparison

Consider a set of models $\{M_i\}$ with prms $\{\vec{\theta}_i\}$. Define likelihood $p(\mathcal{D}|\vec{\theta}_i, M_i)$, then

$$\underbrace{p(\mathcal{D}|M_i)}_{\text{model evidence}} = \int d\vec{\theta}_i \, p(\mathcal{D}|\vec{\theta}_i, M_i)\, p(\vec{\theta}_i|M_i)$$

Under saddle-point approximation,

$$f(\vec{z}) \Rightarrow p(\mathcal{D}|\vec{\theta}_i, M_i)\, p(\vec{\theta}_i|M_i):$$

$$p(\mathcal{D}|M_i) \simeq p(\mathcal{D}|\vec{\theta}_{i,MAP}, M_i)\, p(\vec{\theta}_{i,MAP}|M_i) \times$$

$$\times \frac{(2\pi)^{M/2}}{|A_i|^{1/2}}, \quad \text{where}$$

M is the # model prms and (in model M_i [strictly speaking, $M \to M_i$])

$$A_i = -\vec{\nabla}_{\vec{\theta}}\vec{\nabla}_{\vec{\theta}}\left[\log\underbrace{\left(p(\mathcal{D}|\vec{\theta}_i, M_i)\, p(\vec{\theta}_i|M_i)\right)}_{Z\, p(\vec{\theta}_i|\mathcal{D}, M_i),\ \text{s.t.}}\right]\Big|_{\vec{\theta}_{i,MAP}} =$$

$$\log(\ldots) = \log p(\vec{\theta}_i|\mathcal{D}, M_i) + \underbrace{\log Z}_{\text{const}(\vec{\theta}_i)}$$

$$= -\vec{\nabla}_{\vec{\theta}}\vec{\nabla}_{\vec{\theta}}\left[\log \underbrace{p(\vec{\theta}_i|\mathcal{D}, M_i)}_{\text{posterior}}\right]\Big|_{\vec{\theta}_{i,MAP}}.$$

Finally,

$$\log p(\mathcal{D}|M_i) \simeq \overbrace{\log p(\mathcal{D}|\vec{\theta}_{i,MAP}, M_i)}^{\log \cdot \mathcal{L}} + \underbrace{\log p(\vec{\theta}_{i,MAP}|M_i) + \frac{M}{2}\log(2\pi) - \frac{1}{2}\log|A_i|}_{\text{"penalty" for model complexity}}$$

Moreover, assume that priors are given by

$$p(\vec{\theta}_i|M_i) = \mathcal{N}(\vec{\theta}_i|\vec{0}, \alpha^{-1}\mathbb{I}) = \frac{\alpha^{M/2}}{(2\pi)^{M/2}} e^{-\frac{1}{2}\vec{\theta}_i \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix} \vec{\theta}_i}$$ as before.

Then $A_i = \underbrace{-\vec{\nabla}\vec{\nabla}\left[\log p(\mathcal{D}|\vec{\theta}_i, M_i)\right]\Big|_{\vec{\theta}_{i,MAP}}}_{\equiv H} - \underbrace{\vec{\nabla}\vec{\nabla}\left[\log p(\vec{\theta}_i|M_i)\right]\Big|_{\vec{\theta}_{i,MAP}}}_{\alpha\mathbb{I}} = H + \alpha\mathbb{I} \simeq H$ if α small or we have lots of data (N is large)

note that $-\log p(\mathcal{D}|\vec{\theta}_i, M_i)$ has $\sum_{n=1}^{N} \ldots$ and $\uparrow$ as $N\uparrow$

we have:

$$\log p(\mathcal{D}|M_i) \simeq \log p(\mathcal{D}|\vec{\theta}_{i,MAP}, M_i) - \frac{\alpha}{2}\vec{\theta}_{i,MAP}^{T}\vec{\theta}_{i,MAP} - \frac{1}{2}\log|H| + \underbrace{-\frac{M}{2}\log(2\pi) + \frac{M}{2}\log\alpha + \frac{M}{2}\log(2\pi)}_{\text{log correction}}$$

same argument as above (α small and/or N large)

in the large-N limit

Finally,

$$H = \sum_{n=1}^{N} H_n = N\underbrace{\langle H\rangle}_{\frac{1}{N}\sum_n H_n} \Rightarrow \log|H| = \log|N\langle H\rangle| = \log[N^M |\langle H\rangle|] =$$

$\Uparrow$ this assumes that the rank of H is M

$$= M\log N + \log|\langle H\rangle|.$$

We obtain:

$$\boxed{\log p(\mathcal{D}|M_i) \simeq \log p(\mathcal{D}|\vec{\theta}_{i,MAP}, M_i) - \underbrace{\frac{M}{2}\log N}_{\text{complexity penalty}}}$$

Bayesian information criterion (BIC)