

Artificial neural networks

- Feedforward NN with one hidden layer:

$$\hat{\mathbf{y}} = \varphi(\mathbf{W}^{(2)}\sigma^{(1)}(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) + \mathbf{b}^{(2)}) = \varphi\left(\sum_{k=1}^K W_{kl}^{(2)} \sigma^{(1)}\left(\sum_{j=1}^J W_{jk}^{(1)} x_j + b_j^{(1)}\right) + b_k^{(2)}\right)$$

\mathbf{x} = input layer

$\hat{\mathbf{y}}$ = output prediction layer

θ = parameters to estimate = $\{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \mathbf{W}^{(2)}, \mathbf{b}^{(2)}\}$

$$\sigma(\mathbf{z}) = \begin{cases} \max(\mathbf{0}, \mathbf{z}) & \text{relu, defacto standard} \\ (1 + e^{-\mathbf{z}})^{-1} & \text{sigmoid, old school} \\ \text{many} & \text{variations on these and others} \end{cases}$$

$$\varphi(\mathbf{z}) = \begin{cases} \text{htan } \mathbf{z} & \text{regression} \\ \frac{e^{\mathbf{z}}}{\sum_{\mathbf{z}} e^{\mathbf{z}}} & \text{classification} \end{cases}$$

NN parameter estimation for regression

- Model: $\mathbf{Y} = \hat{\mathbf{Y}} + \epsilon = f(\mathbf{X}; \boldsymbol{\theta}) + \epsilon$ where $f(\mathbf{X}; \boldsymbol{\theta})$ expresses our neural network

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$$\boldsymbol{\epsilon} \sim N(\mathbf{Y} - f(\mathbf{X}; \boldsymbol{\theta}), \boldsymbol{\Sigma})$$

$$= \sqrt{\frac{1}{(2\pi)^N \det \Sigma}} e^{-\frac{1}{2}(\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}))^T \Sigma^{-1}(\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}))}$$

- Optimization: $\hat{\theta} = \underset{\theta}{\operatorname{argmin}} -\log P(\mathbf{Y} \mid \mathbf{X}; \theta)$

$$:= P(\mathbf{Y} | \mathbf{X}; \boldsymbol{\theta}) \leftarrow \mathcal{L}(\mathbf{D}; \boldsymbol{\theta})$$

$$= \operatorname{argmin}_{\boldsymbol{\theta}} -\log\left(\sqrt{\frac{1}{(2\pi)^N \det \boldsymbol{\Sigma}}} \exp\left[-\frac{1}{2}(\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}))^T \boldsymbol{\Sigma}^{-1}(\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}))\right]\right)$$

$$= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \quad -\frac{1}{2} \log((2\pi)^N \det \boldsymbol{\Sigma}) - \frac{1}{2} (\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}))^T \boldsymbol{\Sigma}^{-1} (\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}))$$

$$= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \quad - \left(\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}) \right)^T \left(\mathbf{X} - f(\mathbf{X}; \boldsymbol{\theta}) \right)$$

$$= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \quad - \sum_{i=1}^M (\mathbf{y}^{(i)} - f(\mathbf{x}^{(i)}; \boldsymbol{\theta}))^T (\mathbf{y}^{(i)} - f(\mathbf{x}^{(i)}; \boldsymbol{\theta}))$$

$$= \underset{\boldsymbol{\theta}}{\operatorname{argmin}} - \sum_{i=1}^M \sum_{j=1}^N (\mathbf{y}_j^{(i)} - f(\mathbf{x}^{(i)}; \boldsymbol{\theta}))_j^2 \quad \leftarrow \text{least squares}$$

→ Σ is diagonal, strictly positive, independent of \mathbf{x} ; it doesn't affect $\hat{\theta}$