

ANALYTICAL GRADIENT OF BNN POTENTIAL ENERGY

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$$f(x, \omega) = b + \sum_{j=1}^H v_j \tanh(a_j + \sum_{i=1}^I u_{ji} x_i)$$

$$L = \prod_{k=1}^N e^{-\frac{w_k(t_k - f(x_k, \omega))^2}{2\sigma^2}}$$

$$\text{Prior}(\omega) = \prod_{i=1}^{n\omega} e^{-\frac{\omega_i^2}{2\sigma_i^2}}$$

$$P = f(x, \omega) * \text{Prior}(\omega)$$

$$U = -\ln P = -\ln(L) - \ln \text{Prior}(\omega)$$

$$U = \frac{1}{2\sigma^2} \sum_{k=1}^N (w_k(t_k - f(x_k, \omega))^2) + \sum_{i=1}^{n\omega} \frac{\omega_i^2}{2\sigma_i^2}$$

$$\nabla_{\omega} U = -\frac{1}{\sigma^2} \sum_{k=1}^N w_k(t_k - f(x_k, \omega)) \nabla_{\omega} f(x_k, \omega)$$

$$\nabla_{\omega} U = \begin{cases} -\frac{1}{\sigma^2} \sum_{k=1}^N w_k(t_k - f(x_k, \omega)) + \frac{b}{\sigma_b} & : b \\ -\frac{1}{\sigma^2} \sum_{k=1}^N w_k(t_k - f(x_k, \omega)) \tanh(a_j + \sum_{i=1}^I u_{ji} x_i) + \frac{v_j}{\sigma_v} & : v_j \\ -\frac{1}{\sigma^2} \sum_{k=1}^N w_k(t_k - f(x_k, \omega)) v_j (1 - \tanh^2(a_j + \sum_{i=1}^I u_{ji} x_i)) + \frac{a_j}{\sigma_a} & : a_j \\ -\frac{1}{\sigma^2} \sum_{k=1}^N w_k(t_k - f(x_k, \omega)) v_j x_{ik} (1 - \tanh^2(a_j + \sum_{i=1}^I u_{ji} x_{ik})) + \frac{u_{ji}}{\sigma_u} & : u_{ji} \end{cases}$$