

# Hyperparameter optimization with Lagrange multipliers

Henrik Lund Mortensen

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**Problem:**

Minimize  $E_{\text{val}}(\mathbf{w})$  with respect to  $\sigma$ , where  $\mathbf{w} = (\mathbf{K} + \gamma \frac{N}{2})^{-1} \mathbf{Y}$

Instead of  $E_{\text{val}}(\tilde{\mathbf{w}})$  we minimize the Lagrangian

$$\mathcal{L}(\mathbf{w}, \mathbf{p}, \sigma) = E_{\text{val}}(\mathbf{w}) + \mathbf{p} \cdot \left( \frac{2}{N} (\mathbf{K}\mathbf{w} - \mathbf{Y}) + \gamma \mathbf{w} \right) \quad (1)$$

The Lagrangian is minimized by setting all partial derivative to zero

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = 0 \quad , \quad \frac{\partial \mathcal{L}}{\partial \mathbf{p}} = 0 \quad , \quad \frac{\partial \mathcal{L}}{\partial \sigma} = 0 \quad (2)$$

The derivative with respect to the multiplier gives

$$0 = \frac{\partial \mathcal{L}}{\partial \mathbf{p}} = \frac{2}{N} (\mathbf{K}\mathbf{w} - \mathbf{Y}) + \gamma \mathbf{w} \quad (3)$$

$$\mathbf{w} = \left( \mathbf{K} + \gamma \frac{N}{2} \right)^{-1} \mathbf{Y}, \quad (4)$$

which is just the condition on  $\mathbf{w}$ . The derivative of  $\mathcal{L}$  with respect to  $\mathbf{w}$  gives

$$0 = \frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \frac{\partial E_{\text{val}}(\mathbf{w})}{\partial \mathbf{w}} + \mathbf{p} \cdot \left( \gamma + \frac{2}{N} \mathbf{K} \right) \quad (5)$$

$$\mathbf{p} = - \frac{\partial E_{\text{val}}(\mathbf{w})}{\partial \mathbf{w}} \left( \gamma + \frac{2}{N} \mathbf{K} \right)^{-1} \quad (6)$$