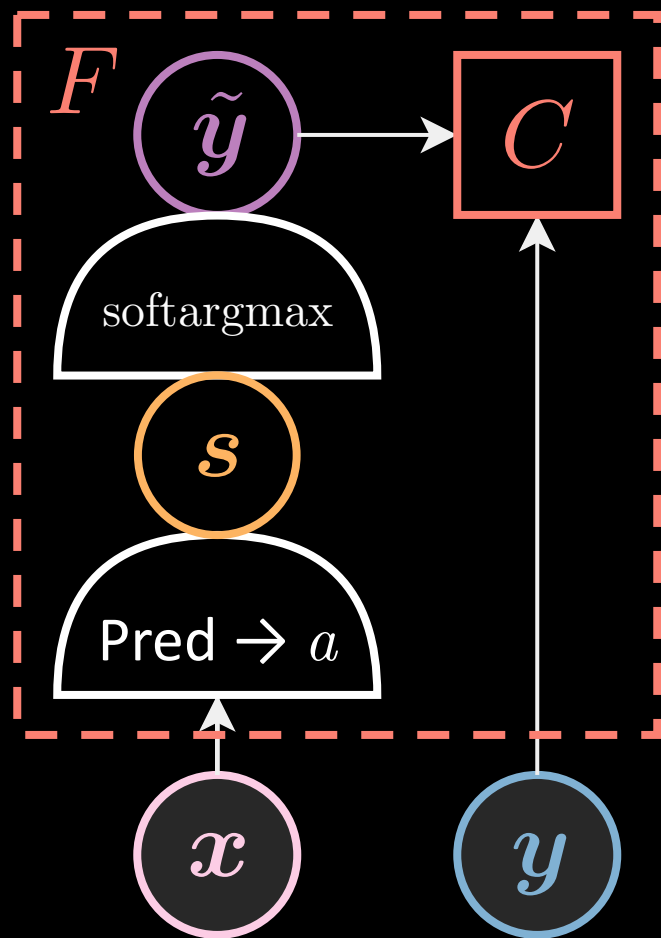


Cross-entropy vs. negative-linear-output

Two possible energy perspective for a classifier

$$F(\boldsymbol{x}, \boldsymbol{y}) = C(\tilde{\boldsymbol{y}}, \boldsymbol{y})$$

Cross-entropy



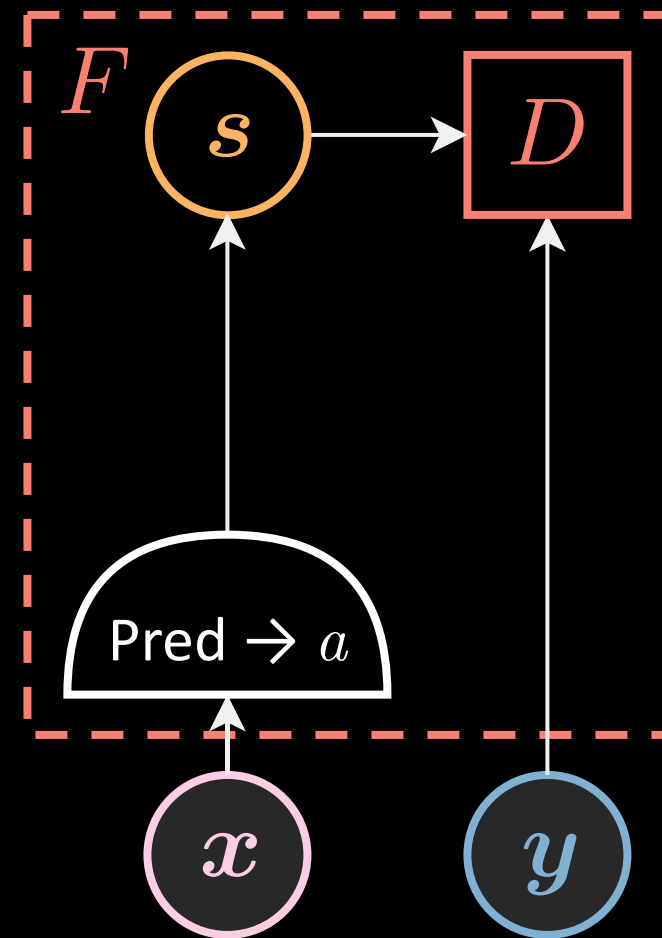
$$\begin{aligned} L[F(\boldsymbol{x}, \mathcal{Y}), \boldsymbol{y}] &= \\ &= F(\boldsymbol{x}, \boldsymbol{y}) + \\ &\log \sum_{\boldsymbol{y}' \in \mathcal{Y}} \exp[-F(\boldsymbol{x}, \boldsymbol{y}')] \end{aligned}$$

$$C(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = -\log(\boldsymbol{y}^\top \tilde{\boldsymbol{y}})$$

$$D(\boldsymbol{y}, \boldsymbol{s}) = -\boldsymbol{y}^\top \boldsymbol{s}$$

$$F(\boldsymbol{x}, \boldsymbol{y}) = D(\boldsymbol{y}, \boldsymbol{s})$$

Negative linear output



Negative linear output energy $F(\mathbf{x}, \mathbf{y}) = D(\mathbf{y}, \mathbf{s})$

$$D(\mathbf{y}, \mathbf{s}) = -\mathbf{y}^\top \mathbf{s} \qquad D(\mathcal{Y}, \mathbf{s}) = -\mathbf{s} \quad \begin{array}{l} \text{negative} \\ \text{linear output} \end{array}$$

$$L[F(\mathbf{x}, \mathcal{Y}), \mathbf{y}] = -\frac{1}{\beta} \log(\mathbf{y}^\top \text{softargmin}_\beta[F(\mathbf{x}, \mathcal{Y})]) \quad \begin{array}{l} \text{loss} \\ \text{functional} \end{array}$$

$$\text{softargmin}_\beta[F(\mathbf{x}, \mathcal{Y})] \doteq \frac{\exp[-\beta F(\mathbf{x}, \mathcal{Y})]}{\sum_{\mathbf{y}' \in \mathcal{Y}} \exp[-\beta F(\mathbf{x}, \mathbf{y}')]}$$

$$L[F(\mathbf{x}, \mathcal{Y}), \mathbf{y}] = F(\mathbf{x}, \mathbf{y}) + \boxed{\frac{1}{\beta} \log \sum_{\mathbf{y}' \in \mathcal{Y}} \exp[-\beta F(\mathbf{x}, \mathbf{y}')]}$$

$-\text{softmin}_{\beta}[F(\mathbf{x}, \mathcal{Y})]$

Gradients wrt the free energy $\hat{\mathbf{y}} \mid \mathbf{x} \in \mathcal{Y} \setminus \mathbf{y} \mid \mathbf{x}$

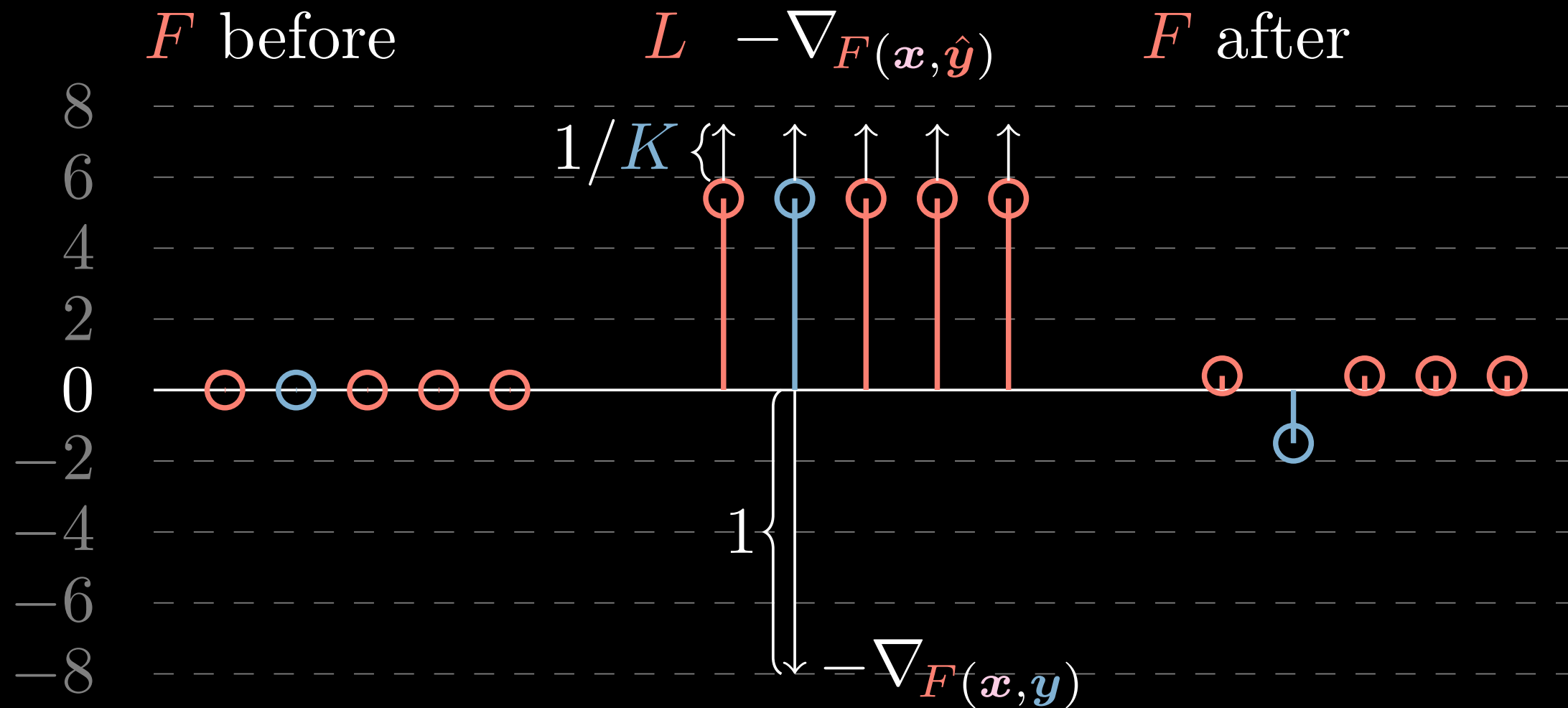
$$L[F(\mathbf{x}, \mathcal{Y}), \mathbf{y}] = F(\mathbf{x}, \mathbf{y}) - \text{softmax}_{\beta}[F(\mathbf{x}, \mathcal{Y})]$$

$$\begin{aligned} \nabla_{F(\mathbf{x}, \mathbf{y})} L[F(\mathbf{x}, \mathcal{Y}), \mathbf{y}] &= 1 - \frac{\exp[-\beta F(\mathbf{x}, \mathbf{y})]}{\sum_{\mathbf{y}' \in \mathcal{Y}} \exp[-\beta F(\mathbf{x}, \mathbf{y}')] } = \\ &= 1 - \mathbb{P}_{\mathbf{w}}^{\beta}(\mathbf{y} \mid \mathbf{x}) = 1 - \mathbf{y}^{\top} \tilde{\mathbf{y}} \end{aligned}$$

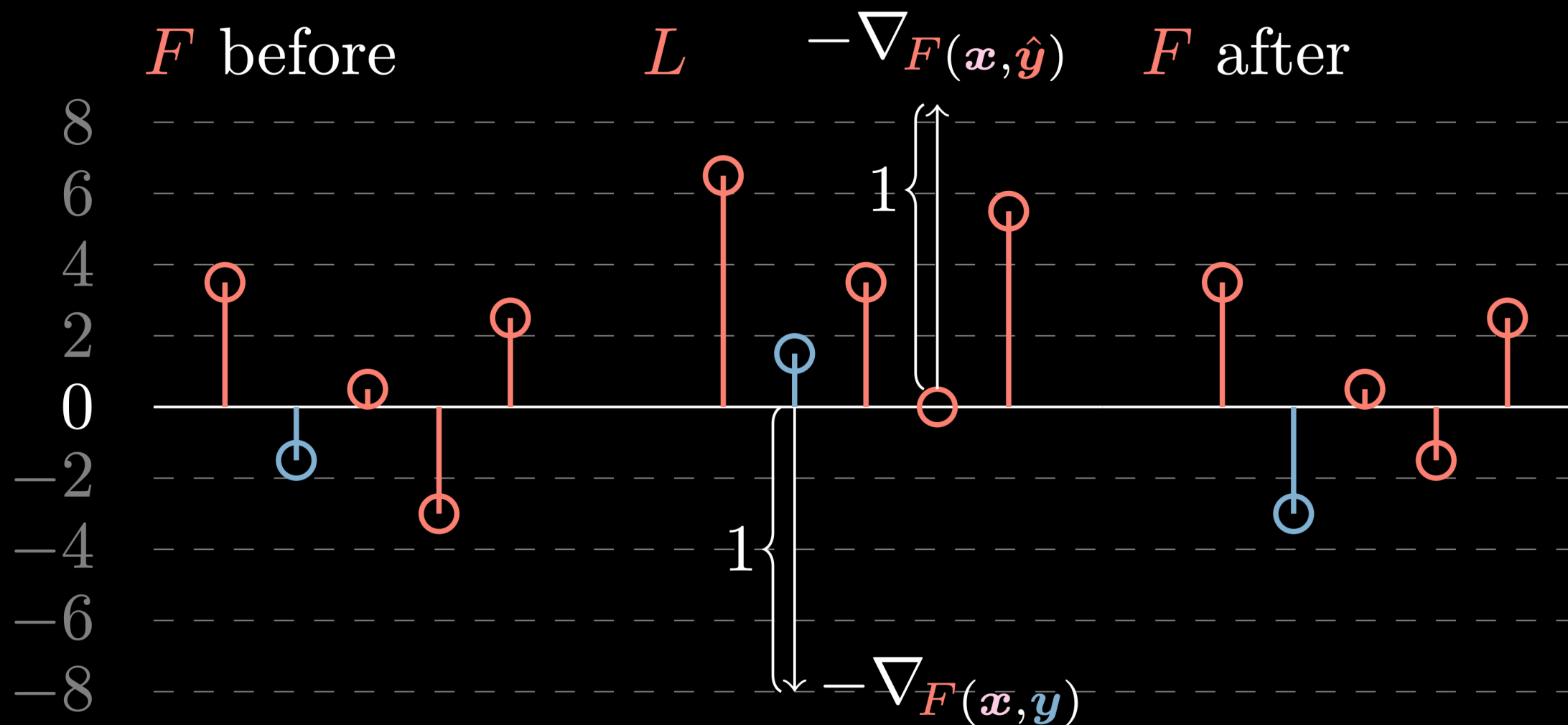
$$\nabla_{F(\mathbf{x}, \hat{\mathbf{y}})} L[F(\mathbf{x}, \mathcal{Y}), \mathbf{y}] = 0 - \mathbb{P}_{\mathbf{w}}^{\beta}(\hat{\mathbf{y}} \mid \mathbf{x}) = -\hat{\mathbf{y}}^{\top} \tilde{\mathbf{y}}$$

$$\begin{aligned} \mathbb{P}_{\mathbf{w}}^{\beta}(\mathbf{y}' \mid \mathbf{x}) &\doteq \text{softmax}_{\beta}[F(\mathbf{x}, \mathcal{Y})]^{\top} \mathbf{y}' & \nabla_{F(\mathbf{x}, \mathcal{Y})} L &= \\ & & &= \mathbf{y} - \tilde{\mathbf{y}} \end{aligned}$$

$$\nabla_{F(x, \mathcal{Y})} L[F(x, \mathcal{Y}), y] = y - \tilde{y} \quad F(x, \mathcal{Y}) = \mathbf{0}$$



$$\nabla_{F(x, y)} L[F(x, y), y] = y - \tilde{y} \quad \beta \rightarrow +\infty$$



$$\nabla_{F(x, \mathcal{Y})} L[F(x, \mathcal{Y}), y] = y - \tilde{y}$$

