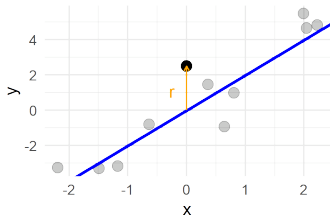
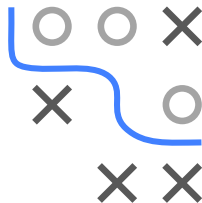


Introduction to Machine Learning

Advanced Risk Minimization Pseudo-Residuals



Learning goals

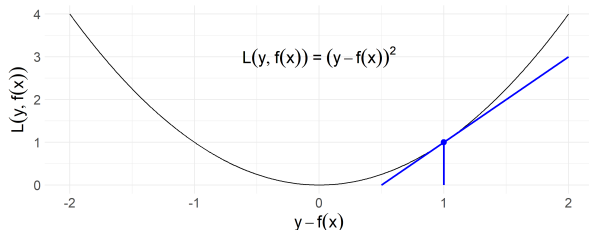
- Concept of pseudo-residuals
- PRs for common losses

PSEUDO-RESIDUALS

- In regression, residuals are defined as $r(\mathbf{x}) := y - f(\mathbf{x})$
- Generalize concept to **pseudo-residuals**:

$$\tilde{r}(\mathbf{x}) := -\frac{dL(y, f(\mathbf{x}))}{df(\mathbf{x})}$$

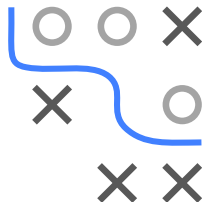
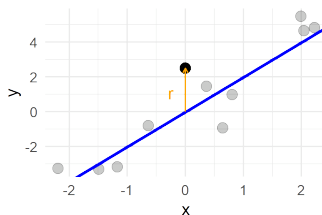
- If we wiggle $f(\mathbf{x})$, how much does L change?
- Can be used for score-based classifiers and other models
- Note that $\tilde{r}(\mathbf{x})$ depends on y , $f(\mathbf{x})$ and L



BEST POINT-WISE UPDATE

- Assume we have (partially) fitted a model $f(\mathbf{x})$ to data \mathcal{D}
- Assume we could update $f(\mathbf{x})$ point-wise as we like
- Under squared loss, for a fixed $\mathbf{x} \in \mathcal{X}$, the best point-wise update is the direction of the residual $r(\mathbf{x}) = y - f(\mathbf{x})$

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + r(\mathbf{x})$$

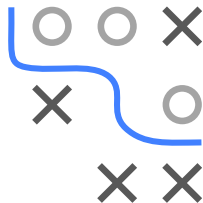
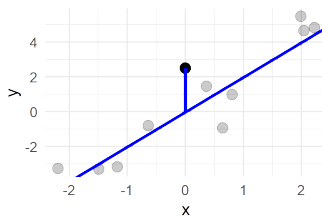


BEST POINT-WISE UPDATE

- Assume we have (partially) fitted a model $f(\mathbf{x})$ to data \mathcal{D}
- Assume we could update $f(\mathbf{x})$ point-wise as we like
- Under squared loss, for a fixed $\mathbf{x} \in \mathcal{X}$, the best point-wise update is the direction of the residual $r(\mathbf{x}) = y - f(\mathbf{x})$

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + r(\mathbf{x})$$

- Point-wise error at this specific \mathbf{x} becomes 0

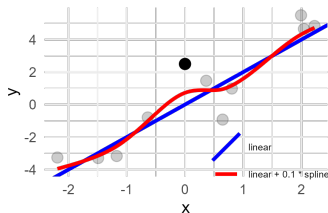
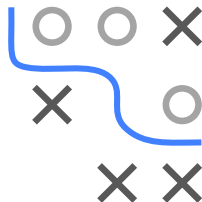


BEST POINT-WISE UPDATE

- Assume we have (partially) fitted a model $f(\mathbf{x})$ to data \mathcal{D}
- Assume we could update $f(\mathbf{x})$ point-wise as we like
- Under squared loss, for a fixed $\mathbf{x} \in \mathcal{X}$, the best point-wise update is the direction of the residual $r(\mathbf{x}) = y - f(\mathbf{x})$

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + r(\mathbf{x})$$

- (In gradient boosting, which we cover later, we don't do point-wise updates but “smoothly distort” f so we generalize)



APPROXIMATE BEST POINT-WISE UPDATE

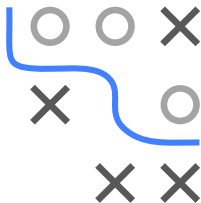
- Best local change of f at \mathbf{x} to reduce loss most:

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) - \frac{dL(y, f(\mathbf{x}))}{df(\mathbf{x})}$$

- This is effectively the PR

$$f(\mathbf{x}) \leftarrow f(\mathbf{x}) + \tilde{r}(\mathbf{x})$$

- (Such iterative updates of f like a loss-reducing GD in function space is the major underlying idea of GB)



GD IN ML AND PSEUDO-RESIDUALS

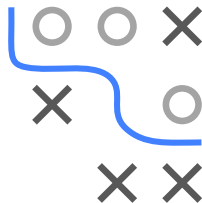
- In GD, we move in the direction of the negative gradient by updating the parameters:

$$\theta^{[t+1]} = \theta^{[t]} - \alpha^{[t]} \cdot \nabla_{\theta} \mathcal{R}_{\text{emp}}(\theta)|_{\theta=\theta^{[t]}}$$

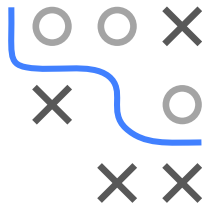
- Using the chain rule:

$$\begin{aligned}\nabla_{\theta} \mathcal{R}_{\text{emp}}(\theta) &= \sum_{i=1}^n \frac{dL(y^{(i)}, f(\mathbf{x}))}{df(\mathbf{x})} \bigg|_{f=f(\mathbf{x}^{(i)} | \theta)} \cdot \nabla_{\theta} f(\mathbf{x}^{(i)} | \theta) \\ &= - \sum_{i=1}^n \tilde{r}^{(i)} \cdot \nabla_{\theta} f(\mathbf{x}^{(i)} | \theta).\end{aligned}$$

- Update is loss-optimal directional change of model output and a loss-independent derivative of $f(\mathbf{x})$
- This is a flexible, nearly loss-independent variant of GD



PSEUDO-RESIDUALS FOR COMMON LOSSES



Loss	Domain of y	Pseudo residual \tilde{r}
Squared loss	$y \in \mathbb{R}$	$y - f(\mathbf{x})$
Bernoulli loss	$y \in \{0, 1\}$	$y - s(f(\mathbf{x})) = y - \pi(\mathbf{x})$
Multinomial loss	$y \in \{1, \dots, g\}$	$\mathbb{1}_{\{y=k\}} - \pi_k(\mathbf{x})$
Exponential loss	$y \in \{-1, 1\}$	$y \exp(-yf(\mathbf{x}))$

NB: $\pi(\mathbf{x}) = s(f(\mathbf{x})) = \frac{\exp(f(\mathbf{x}))}{1 + \exp(f(\mathbf{x}))}$ is the (sigmoidal) logistic function,
and $\pi_k(\mathbf{x})$ its multi-class generalization, the softmax