A12:Tackling Distribution Shifts via Test-Time Adaptation and Optimization

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Training is Optimization

Supervised learning

- n observations: $\big(x_i \in \mathbb{R}^d, y_i \in \{-1, +1\}\big)$, $i = 1, \ldots, n$.
- Prediction function: $h(x_i; w) \in \mathbb{R}$ parametrized by $w \in W$.

x_1 x_2 x_3 x_4 x_5 x_6

$y_1 = 1$ $y_2 = 1$ $y_3 = 1$ $y_4 = -1$ $y_5 = -1$ $y_6 = -1$

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Regularized Empirical Risk

$$\min_{w \in W} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell(x_i, y_i; h(x_i; w))}_{\text{Empirical Risk}} + \underbrace{\lambda \phi(w)}_{\text{Regularization}}$$

Mathematical Background and Gradient Flow

Review: Calculus

(**Derivative**) For a function $g(\cdot) : \mathbb{R} \to \mathbb{R}$ and $x \in \mathbb{R}$, consider

$$\lim_{\delta \to 0} \frac{g(x+\delta) - g(x)}{\delta}.$$

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The function $g(\cdot)$ is said to be "differentiable" if this limit exits for all $x \in \mathbb{R}$. In that case, the limit is called the "derivative" of $g(\cdot)$.

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We denote the derivative as

(**Gradient**) For a differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^d$, the gradient is

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_d} \end{bmatrix},$$

where

$$\frac{\partial f}{\partial x_1} = \lim_{\delta \to 0} \frac{f(x_1 + \delta; x_2; \dots; x_d) - f(x_1; x_2; \dots; x_d)}{\delta}.$$

Definition

(**Hessian**) For a twice continuously differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ and $\mathbf{x} \in \mathbb{R}^d$, the Hessian matrix of $f(\cdot)$ at $\mathbf{x}$ is defined by

$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

Exercise

Let $f\colon \mathbb{R}^2 \to \mathbb{R}$ be defined by $f(\mathbf{x}) = x_1^2 x_2$. Then

$\nabla f(\mathbf{x}) =$

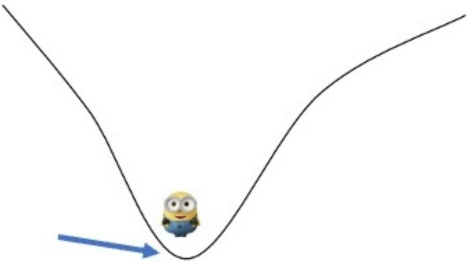
and

$\nabla^2 f(\mathbf{x}) =$

Convergence Rate

Finding the minimizer of a function

$$\min_{x \in \mathbb{R}^d} f(x) \tag{1}$$



Optimality Gap

Definition

(**Optimality Gap**): Given a function f such that $f : \mathbb{R}^d \to \mathbb{R}$, the optimality gap is the difference between the value of f at $\mathbf{x}_k \in \mathbb{R}^d$ at some time point k and the optimal value, i.e.

$$f(\mathbf{x}_k) - \min_{\mathbf{x}} f(\mathbf{x})$$

Gradient Descent

$\min_{x \in \mathbb{R}^d} f(x)$.

Input: an initial point $\mathbf{x}_0 \in \textbf{dom } f$ and step size η.
for $k = 1$ to K **do**
  $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k - \eta \nabla f(\mathbf{x_k})$
end for
Return $\mathbf{x}_{k+1}$.

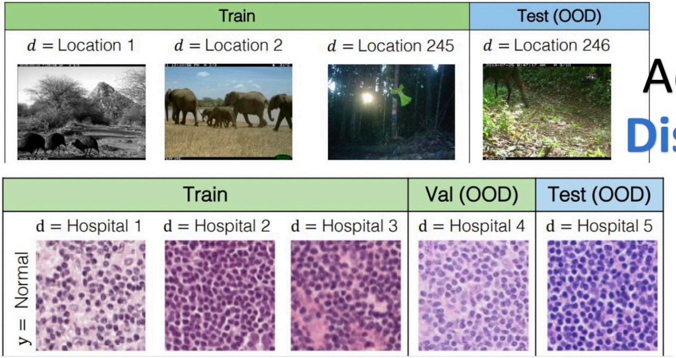
(**Gradient Flow**): Let $f\colon \mathbb{R}^d \to \mathbb{R}$ be a smooth function. Gradient flow is a smooth curve $\mathbf{x} : \mathbb{R} \to \mathbb{R}^d$ such that

$$\frac{d\mathbf{x}(t)}{dt} = -\nabla f(\mathbf{x}(t))$$

Gradient Flow is Gradient Descent as $\eta \to 0$

Our project:
Tackling Distribution Shifts via Test-Time Adaptation and Optimization

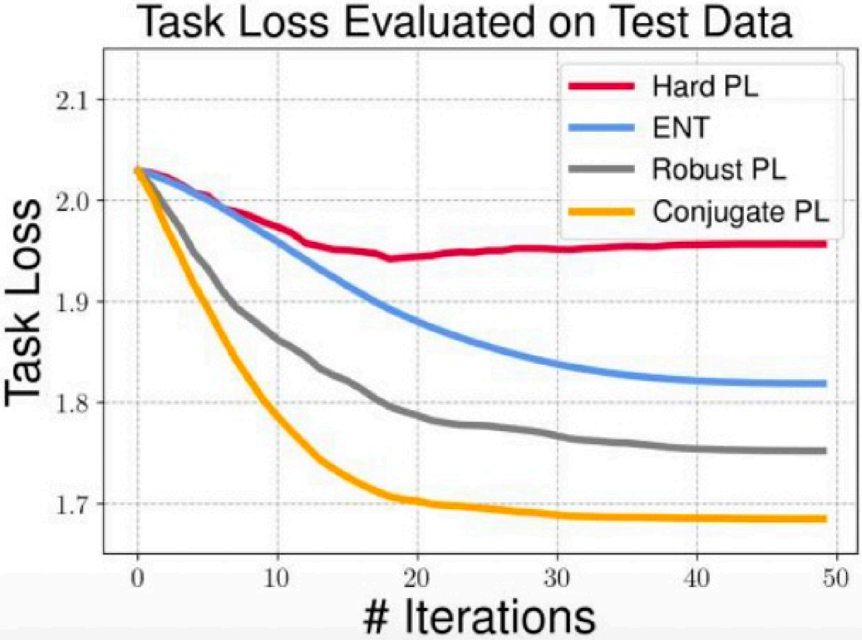
Machine learning has been used widely in Data Science and Engineering



Needs Adaptation Distribution Shifts

Source: Wilds: A Benchmark of in-the-Wild Distribution Shifts. Koh, Sagawa, et al. ICML 2021

Given a source model, adapt the model to a new domain, by using un-labeled samples of data from the new domain.


Task Loss Evaluated on Test Data
Hard PL
ENT
Robust PL
Conjugate PL
Task Loss
2.1
2.0
1.9
1.8
1.7
0
10
20
30
40
50
Iterations

https://docs.google.com/document/d/
1nEa5PQowFBSJhRoUYPjrQ-NKL4G6Qz5VCiv8AjwMQCc/edit