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

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Training is Optimization

Supervised learning

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



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

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Regularized Empirical Risk

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

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Mathematical Background and Gradient Flow

(**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

$$abla f(\mathbf{x}) = egin{bmatrix} rac{\partial f}{\partial x_1} \ rac{\partial f}{\partial x_2} \ dots \ rac{\partial f}{\partial x_d} \end{bmatrix},$$

where

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



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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

$$\nabla^{2} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^{2} f}{\partial x_{1}^{2}} & \frac{\partial^{2} f}{\partial x_{1} \partial x_{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{1} \partial x_{d}} \\ \frac{\partial^{2} f}{\partial x_{2} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{2}^{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{2} \partial x_{d}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{2} f}{\partial x_{d} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{d} \partial x_{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{d}^{2}} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

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Exercise

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

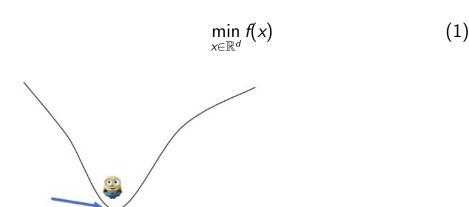
$$\nabla f(\mathbf{x}) =$$

and

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

Convergence Rate

Finding the minimizer of a function



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

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

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



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

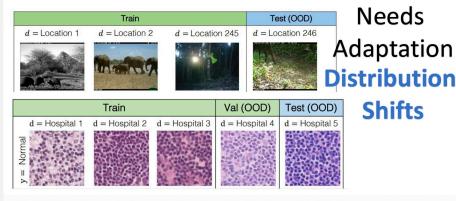
$$\frac{d\mathbf{x}(t)}{dt} = -\nabla f(\mathbf{x}(t))$$

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

Our project:

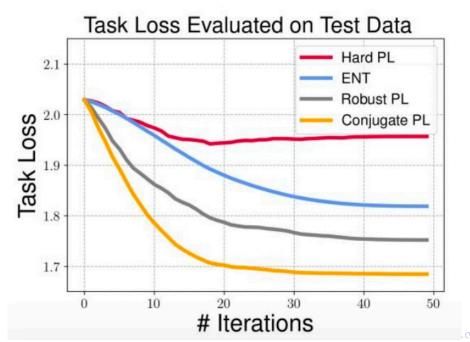
Tackling Distribution Shifts via Test-Time Adaptation and Optimization

Machine learning has been used widely in Data Science and Engineering



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.



Research Group Meeting Schedule https://docs.google.com/document/d/ 1nEa5PQowFBSJhRoUYPjrQ-NKL4G6Qz5VCiv8AjwMQCc/edit