Towards Reciprocal Learning Theory

Generalizing From Self-Selected Samples

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2nd Workshop on Learning Under Weakly Structured Information Tübingen

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Can Reciprocal Learning Converge?

Can Reciprocal Learning Generalize?





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Motivating Example: Self-Training¹



Figure 1: Sketch of Self-Training for Binary Classification

¹Other names: Pseudo-Labeling, Self-Labeling. Julian Rodemann (LMU) 4/28

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Motivation

- Growing interest in experimental design and subsampling²
- We demonstrate that a wide range of (online) learning algorithms *implicitly* design experiments
- reciprocal relationship between data and parameters: These algorithms not only learn parameters from data, but also vice versa
 - self-training (semi-supervised learning)
 - active learning
 - boosting
 - multi-armed bandits
 - superset learning
 - Bayesian optimization
 - **...**

²(Lang, Vijayaraghavan, and Sontag 2022; Liu et al. 2023; Malte Nalenz, Rodemann, and Thomas Augustin 2024; Pooladzandi, Davini, and Mirzasoleiman 2022; Rodemann 2024; Rodemann, Fischer, et al. 2022; Stolz 2023; Yin et al. 2024) Julian Rodemann (LMU) 5/28 7 April 2025 (@LUWSI)

A Visual Perspective



Figure 2: (a) Classical statistical learning fits a model from the model space (restricted by red curve) to a realized sample from the sample space (blue-grey), see Hastie, Tibshirani, and Friedman 2009, Figure 7.2. (b) In reciprocal learning, the sample changes *in response to* the model fit.

What's a fit?

Definition (Risk)

Let $\theta \in \Theta$ a parameter vector. The **risk** of θ on $Z = (X, Y) \sim P$ is

$$\mathscr{R}(P,\theta) := \mathbb{E}_P\left[\ell(Y,X,\theta)\right] = \int_{\mathscr{Z}} \ell(y,x,\theta) \mathrm{d}P(z),$$

where $\ell: \mathcal{Y} \times \mathcal{X} \times \Theta \to \mathbb{R}$ is a loss function and $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$.

Definition (Empirical Risk Minimizer)

Denote by $(x_1, y_1), \ldots, (x_n, y_n)$ a sample with empirical law $\hat{\mathbb{P}}_0$. Call

$$\hat{\theta}_t \in \operatorname*{arg\,min}_{\theta \in \Theta} \mathcal{R}\left(\hat{\mathbb{P}}_0, \theta\right) = \operatorname*{arg\,min}_{\theta} \frac{1}{n} \sum_{i=1}^n \ell(y_i, x_i, \theta)$$

the **empirical risk minimizer** in iteration $t \in \{1, ..., T\}$.

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Reciprocal Learning

Call an algorithm reciprocal if ...

- 1. ... it performs empirical risk minimization (ERM) \ldots
- 2. ... iteratively ...
- 3. ... on a sample that depends ...
 - \blacksquare ... on the previous ERM solution ...
 - ... and the previous sample.

Reciprocal Learning

Definition (Sample Adaptation)

Denote by Θ a parameter space and by \mathscr{P} a space of (joint) probability distributions of X and Y. Call

$$f_s:\begin{cases} \Theta \times \mathcal{P} & \to \mathcal{P} \\ (\hat{\theta}_t, \hat{\mathbb{P}}_t(Y, X)) & \mapsto \hat{\mathbb{P}}_{t+1}(Y, X) \end{cases}$$

the sample adaptation function.

simple example

Reciprocal Learning

Definition (Reciprocal Learning)

With f_s , Θ , \mathcal{P} , X, and Y as above, we define

$$R:\begin{cases} \Theta \times \mathscr{P} & \to \Theta \times \mathscr{P}; \\ (\hat{\theta}_t, \hat{\mathbb{P}}_t) & \mapsto (\hat{\theta}_{t+1}, \hat{\mathbb{P}}_{t+1}) \end{cases}$$

as reciprocal learning, where

$$\hat{\mathbb{P}}_{t+1} = f_s(\hat{\theta}_t, \hat{\mathbb{P}}_t)$$

and

$$\hat{\theta}_{t+1} = \operatorname*{arg\,min}_{\theta \in \Theta} \mathcal{R}(\hat{\mathbb{P}}_{t+1}, \theta)$$

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Yes, it can!



Figure 3: Idea: Bound the change in the data (purple) by the change in the model (yellow).

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Convergence of Reciprocal Learning

Theorem (Convergence of Reciprocal Learning, Informal)

If the sample adaptation f_s is sufficiently Lipschitz (w.r.t. Wasserstein-2 on \mathcal{P} and L2 on Θ) and the loss is strongly convex and continuously differentiable, the iterates $R_t = (\theta_t, \mathbb{P}_t)$ of reciprocal learning R converge to the limit (θ_c, \mathbb{P}_c) point-wise at a linear rate.

Proof idea:

- \blacksquare Show that $R:\Theta\times\mathcal{P}\to\Theta\times\mathcal{P}$ is a contraction
- \blacksquare Convergence is a fixed-point condition on R
- Apply Banach fixed-point theorem

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Sufficient Conditions for Lipschitz-Continuity of f_s

• When is the sample adapation sufficiently Lipschitz?

- \blacksquare continuous predictions of y
- \blacksquare regularized or randomized selection of x

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Regularized Data Selection



Figure 4: Data regularization is symmetrical to classical model regularization, see illustration in "The Elements of Statistical Learning" Hastie, Tibshirani, and Friedman 2009, Figure 7.2.

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Some Corollaries



Figure 5: Reciprocal Learning generalizes (left) machine learning algorithms. Corollaries (right) of convergence results give rise to theory-informed bandits, active learning, self-training etc. algorithms that shall converge.

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References: Reciprocal Learning



Summary:



Julian Rodemann, Christoph Jansen, Georg Schollmeyer (2024). Reciprocal Learning, **First Workshop on Learning Under Weakly Structured Information (LUWSI)**, Munich.

Julian Rodemann, Christoph Jansen, Georg Schollmeyer (2024). Reciprocal Learning, Advances in Neural Information Processing Systems (NeurIPS), Vancouver.



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Summary



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Figure 6: Sample Space



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Figure 7: Bound on Wasserstein distance between law \mathbb{P} and *i.i.d.* sample $\hat{\mathbb{P}}_0$: $W_p(\mathbb{P}, \hat{\mathbb{P}}_0) \leq \beta_0$ (Fournier and Guillin 2015)

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Figure 8: Reciprocal distortion bound $W_p(\hat{\mathbb{P}}_0, \hat{\mathbb{P}}_T) \leq \beta_T$

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Lemma (Reciprocal Distortion Bound)

Let $\hat{\mathbb{P}}_T$ be the empirical distribution of training data at iteration T in reciprocal learning and $\hat{\mathbb{P}}_0$ the initial one. Denote by $W_p(\cdot, \cdot)$ the p-Wasserstein distance and by $\sup_{z,z'} d_{\mathcal{I}}(z,z')^p < \infty$ the diameter bound. It holds

$$W_p(\hat{\mathbb{P}}_0, \hat{\mathbb{P}}_T) \leq \frac{L_s^T - 1}{L_s - 1} \frac{\sup_{z, z'} d_{\mathcal{Z}}(z, z')^p}{n} := \beta_T,$$

where $0 < L_s < 1$ is the Lipschitz constant of the sample adaptation function f_s .

Observe
$$\beta_{\infty} = \frac{\sup_{z,z'} d_{\mathcal{Z}}(z,z')^p}{(1-L_s)n}$$
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Figure 9: Wasserstein Ball for Reciprocal Learning

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Figure 10: Wasserstein Ball for Reciprocal Learning

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Generalization Bounds for Reciprocal Learning

Theorem (Generalization Gap)

Assume Θ is compact. Let $\hat{\theta}_c$ be the solution of reciprocal learning with corresponding $\hat{\mathbb{P}}_c$. It holds

$$\mathscr{R}(\mathbb{P}, \hat{\theta}_c) \le \mathscr{R}(\hat{\mathbb{P}}_c, \hat{\theta}_c) + L_{\ell} \underbrace{\left(\frac{\log\left(4C_a/\delta\right)}{C_b n}\right)^{p/d}}_{\beta_0} + L_{\ell} \underbrace{\frac{\sup_{z, z'} d_{\mathcal{Z}}(z, z')^p}{(1 - L_s)n}}_{\beta_{\infty}}$$

with probability of at least $1 - \delta$ and Lipschitz-constant L_{ℓ} of the loss. Constants C_a, C_b and dimension d are properties of \mathcal{Z} .

Generalization Bounds for Reciprocal Learning

Theorem (Excess Risk Bound, Informal)

Assume Θ is compact. The excess risk $\mathscr{R}(\mathbb{P}, \hat{\theta}_c) - \inf_{\theta \in \Theta} \mathscr{R}(\mathbb{P}, \theta)$ of reciprocal learning is upper bounded with high probabiliy

Proof Idea:

- Bound $\mathcal{R}(\mathbb{P},\hat{\theta}_c)-\mathcal{R}(\hat{\mathbb{P}}_0,\hat{\theta}_c)$ via Kantorovich-Rubinstein lemma
- Tricky part: bound $\mathcal{R}(\hat{\mathbb{P}}_0,\hat{\theta}_c) \mathcal{R}(\hat{\mathbb{P}}_0,\hat{\theta}_0)$
- Bound $\mathscr{R}(\hat{\mathbb{P}}_0, \hat{\bar{\theta}}_0) \inf_{\theta \in \Theta} \mathscr{R}(\mathbb{P}, \theta)$ via a standard symmetrization argument

Generalization Bounds for Reciprocal Learning

Theorem (Excess Risk Bound)

Assume Θ is compact. The excess risk $\mathcal{R}(\mathbb{P}, \hat{\theta}_c) - \mathcal{R}_{\Theta}$ of reciprocal learning is upper bounded by

$$L_{\ell} \left(\frac{\log \left(4C_a/\delta\right)}{C_b n} \right)^{p/d} + \frac{(1+L_a)L_{\ell} \sup_{z,z'} d_{\mathcal{I}}(z,z')^p}{n(1-L_s \max\{1,\frac{\kappa}{\gamma}\})} + \frac{1}{\sqrt{n}} \left(24\mathfrak{C}(\mathcal{F}) + \sqrt{2\ln(1/\delta)} \right),$$

with probability greater or equal than $1 - \frac{\delta}{2}$, where C_a, C_b are again constants depending on p, d, and $\sup_{z,z'} d_{\mathcal{Z}}(z,z')$, L_ℓ is the Lipschitz-constant of the loss, κ and γ are from conditions 2 and 3. L_a shall denote the Lipschitz-constant of $\mathcal{P} \to \Theta : P \mapsto \arg\min_{\theta \in \Theta} \mathscr{R}(P, \theta)$. $\mathfrak{C}_{L_2}(\mathcal{F})$ is the covering entropy integral of a hypothesis class $\mathcal{F} := \{f_\theta : \mathcal{X} \to \mathcal{Y} \mid \theta \in \Theta\}$ with $f_\theta \neq f_{\theta'}$ for $\theta \neq \theta'$.

Anytime Valid Bounds

- What if we stop earlier?
- Good news: Bounds still hold for compact Θ if data selection is regularized (strong convexity of loss not required)

Contents

Recap: Reciprocal Learning

Can Reciprocal Learning Converge?

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Summary

- Reciprocal learning fruitfully generalizes active learning, self-training, multi-armed bandits, Bayesian optimization, superset learning, etc.
- Reciprocal learning converges, if change in sample is bounded by the change in model (Lipschitz)
- This can be achieved through *data regularization*
- Generalization requires "good" initial sample and "smooth"/"very continuous" sample adaptation
- Anytime valid bounds allow for stopping criteria with generalization guarantee

Summary

GENERALIZATION BOUNDS FOR RECIPROCAL LEARNING	
PROS	CONS
Holds for many learning (active learning, bandits, self- training, boosting etc.)	Holds for many learning paradigms (active learning, bandits, self- training, boosting etc.)

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Assume $\mathcal{Y} = \{0, 1\}$ and only one data point being added to a sample of size n.

$$\hat{\mathbb{P}}_{t+1}(Y=1, X=x)$$

$$= \frac{1(x = \boldsymbol{v}(\theta)) \cdot \boldsymbol{\Sigma}(\boldsymbol{v}(\theta), \theta) + n \,\hat{\mathbb{P}}_t(Y=1, X=x)}{n+1}$$

where $\mathbf{\mathfrak{U}}: \mathcal{X} \times \Theta \to \{0, 1\}$ is any function that assigns a label y, potentially based on the model θ , to selected x. Let $\mathbf{\mathfrak{U}}$ be any function that selects features x given a model θ .

Reciprocal Learning: Examples

■ label assignment $\mathfrak{L} : \mathcal{X} \times \Theta \to \{0, 1\}$

- Active Learning: Query function $q_y : \mathcal{X} \to \{0, 1\}$
- Self-Training (SSL): prediction function $\hat{y} : \mathcal{X} \times \Theta \rightarrow \{0, 1\}$
- \blacksquare Bandits: $R:\mathcal{A}\to\{0,1\}$ reward function

• criterion $c: \mathcal{X} \times \Theta \to \mathbb{R}$

- Active Learning: acquisition function
- Self-Training (SSL): confidence measures
- Bandits: policy function³

• selection $\boldsymbol{w}: \boldsymbol{\Theta} \to \mathcal{X}$

- Active Learning: $\arg \max_x$
- **Self-Training** (SSL): $\operatorname{arg} \max_x$
- Bandits: Thompson sampling, epsilon-greedy (stochastic); upper confidence bound (deterministic)

back

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³It is often directly defined in terms of action selection probabilities.

- self-training (semi-supervised learning) (Arazo et al. 2020;
 Dietrich, Rodemann, and Christoph Jansen 2024; Lee et al. 2013;
 Li et al. 2020; Rizve et al. 2020; Rodemann, Goschenhofer, et al. 2023; Rodemann, Christoph Jansen, et al. 2023)
- active learning
- multi-armed bandits
- Bayesian optimization (Rodemann 2023; Rodemann and Augustin 2024; Rodemann and Thomas Augustin 2021, 2022; Rodemann, Croppi, et al. 2024)
- superset learning (Hüllermeier and Cheng 2015; Rodemann, Kreiss, et al. 2022)

Reciprocal Learning Through a Decision-Theoretic Lense

Think of reciprocal learning as sequential decision-making⁴:

- $t = 1 \ \theta_1$ solves decision problem $(\Theta, \mathbb{A}_{\Theta}, \ell)$
 - a_1 solves decision problem $(\Theta, \mathbb{A}_{\mathcal{X}}, \ell_{\theta_1})$
- $t = 2 \ \theta_2 \text{ solves decision problem } (\Theta, \mathbb{A}_{\Theta}, \ell_{a_1(\theta_1)})$ $a_2 \text{ solves decision problem } (\Theta, \mathbb{A}_{\mathcal{X}}, \ell_{\theta_2})$

$t = 3 \dots$

with Θ the set of states of nature (parameter space) as well as action spaces $\mathbb{A}_{\Theta} = \Theta$ and $\mathbb{A}_{\mathcal{X}} = \mathcal{X}$ (feature space) for parameter and data selection, respectively.

⁴Notably, addressing machine learning problems from a decision-theoretic point of view has received considerable interest recently C. Jansen, M. Nalenz, et al. 2023; C. Jansen, Schollmeyer, and T. Augustin 2018, 2023; C. Jansen, Schollmeyer, H. Blocher, et al. 2023; Christoph Jansen et al. 2024; Rodemann and Hannah Blocher 2024

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Convergence Won't Come For Free

Assumption (Continuous Differentiability in Features)

A loss function $\ell(Y, X, \theta)$ is said to be continuously differentiable with respect to features if the gradient $\nabla_X \ell(Y, X, \theta)$ exists and is α -Lipschitz continuous in θ , x, and y with respect to the L2-norm on domain and codomain.

Assumption (Continuous Differentiability in Parameters)

A loss function $\ell(Y, X, \theta)$ is continuously differentiable with respect to parameters if the gradient $\nabla_{\theta}\ell(Y, X, \theta)$ exists and is β -Lipschitz continuous in θ , x, and y with respect to the L2-norm on domain and codomain.

Convergence Won't Come For Free

Assumption (Strong Convexity)

A loss function $\ell(Y, X, \theta)$ is said to be γ -strongly convex if

$$\ell(y, x, \theta) \ge \ell(y, x, \theta') + \nabla_{\theta} \ell(y, x, \theta')^{\top} (\theta - \theta') + \frac{\gamma}{2} \|\theta - \theta'\|_{2}^{2},$$

for all θ, θ', y, x . If $\gamma = 0$, this assumption is equivalent to convexity. If $\ell(y, x, \theta) = \ell(z, \theta)$ with $z \in \mathbb{Z} = \mathcal{X} \times \mathcal{Y}$, then strong convexity is equivalently characterized by the existence of $\gamma > 0$ such that

$$\forall z \in \mathcal{Z} : \nabla^2_{\theta} \ell(Z, \theta) \ge \gamma.$$

For examples, see Shalev-Shwartz and Ben-David 2014, Chapter 12.

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Conditions for Convergence (ctd.)

Condition (Stochastic Data Selection)

Data is selected stochastically by drawing from a normalized criterion $\frac{\exp(c(x,\theta_t))}{\int_{x'}\exp(c(x',\theta_t))d\mu(x)}.$

Conditions for Convergence II (ctd.)

Condition (Continuous Selection Criterion)

It holds for the decision criterion $c : \mathcal{X} \times \Theta \to \mathbb{R}$ in the decision problem $(\Theta, \mathbb{A}, \ell_{\theta_t})$ of selecting features to be added to the sample that $\nabla_x c(x, \theta)$ and $\nabla_\theta c(x, \theta)$ are bounded from above.

Condition (Linear Selection Criterion)

The decision criterion $c : \mathcal{X} \times \Theta \to \mathbb{R}$ in $(\Theta, \mathbb{A}, \ell_{\theta_t})$ is linear in x and Lipschitz-continuous in θ with a Lipschitz constant L_c that is independent of x.

Condition (Soft Labels Prediction)

The prediction function $\hat{y}: \mathcal{X} \times \Theta \to \{0, 1\}$ on bounded \mathcal{X} gives rise to a non-degenerate distribution of $Y \mid X$ for any θ such that we can consider soft label predictions $p: \mathcal{X} \times \Theta \to [0, 1]$ with $p(x, \theta) = \sigma(g(X, \theta))$ with $\sigma: \mathbb{R} \to [0, 1]$ a sigmoid function. Further assume that the loss is jointly smooth in these predictions. That is, $\nabla_p \ell(y, p(x, \theta))$ exists and is Lipschitz-continuous in x and θ .

We can interpret p as $P_{\theta}(Y \mid X = x)$. In other words, soft labels in the form of probability distributions are available.

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