A consistent algorithmic framework for structured machine learning

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joint work with C. Ciliberto (Imperial College), A. Rudi (INRIA-Paris)
Classic supervised learning

given \{ (x_1, y_1), \ldots, (x_n, y_n) \} find \ f(x_{\text{new}}) \sim y_{\text{new}}

Regression

Binary classification
Structured learning

“A domain of machine learning, in which the prediction must satisfy the additional constraints found in structured data, poses one of machine learning’s greatest challenges: learning functional dependencies between arbitrary input and output domains.”

Structured learning applications

- Image segmentation [2],
- captioning [3],
- speech recognition [4, 5],
- protein folding [6],
- ordinal regression [7],
- ranking [8].
Examples of “structured” outputs

- Finite discrete alphabets (binary/multi-category classification, multilabel),
- strings,
- ordered lists,
- sequences.

Classically only discrete possibly output spaces.
Classical approaches

Likelihood estimation models
- General approaches (Struct-SVM [9], Conditional Random Fields [10]),
- but limited guarantees (generalization bounds).

Surrogate approaches
- Strong theoretical guarantees,
- but ad hoc, e.g. classification [11], multiclass [12], ranking [8]...

We will try to take the best of both!
Outline

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Statistical learning

- $(\mathcal{X} \times \mathcal{Y}, \rho)$ probability space, such that $\rho(x, y) = \rho_X(x)\rho(y|x)$.
- $\Delta : \mathcal{Y} \times \mathcal{Y} \rightarrow [0, \infty)$
(\mathcal{X} \times \mathcal{Y}, \rho) \text{ probability space, such that } \rho(x, y) = \rho_X(x)\rho(y|x).

\Delta : \mathcal{Y} \times \mathcal{Y} \to [0, \infty)

Problem Solve

\[
\min_{f \in \mathcal{Y}^\mathcal{X}} \int d\rho(x, y)\Delta(f(x), y)
\]

given \((x_i, y_i)_{i=1}^n\) i.i.d. samples of \(\rho\).
Empirical risk minimization (ERM)

\[
\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \Delta(f(x_i), y_i)
\]

- Statistically sound

\[
\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \Delta(f(x_i), y_i) - \int d\rho(x, y) \Delta(f(x), y) \right|
\]

- Impractical: how to pick \( \mathcal{F} \subset \mathcal{Y}^\mathcal{X} \) if \( \mathcal{Y} \) is not linear?
Inner risk

Lemma (Ciliberto, Rudi, R. ’17)

Let

\[ f_\ast = \arg\min_{f \in \mathcal{Y}^X} \int d\rho(x, y) \Delta(f(x), y) \]

then

\[ f_\ast(x) = \arg\min_{y \in \mathcal{Y}} \int d\rho(y|x) \Delta(y, y'). \]
Definition (SELF)

The loss function \( \Delta : \mathcal{Y} \times \mathcal{Y} \to [0, \infty) \) is such that there exists

- a real separable Hilbert space \((\mathcal{H}, \langle \cdot, \cdot \rangle)\) and
- maps \(\Psi, \Phi : \mathcal{Y} \to \mathcal{H}\)

such that \(\forall y, y' \in \mathcal{Y}\)

\[
\Delta(y, y') = \langle \Psi(y), \Phi(y') \rangle
\]
Examples of SELF

- In any finite output spaces $|\mathcal{Y}| = T$
  $$\Delta(y, y') = e_y^T V e_{y'}, \quad V \in \mathbb{R}^{T \times T}.$$ 

- Symmetric positive definite loss functions, Kernel Dependency Estimator [16].

- Smooth loss functions with $\mathcal{Y} = [0, 1]^d$.

- Restriction of SELF are SELF, and SELF can be composed.
Structured statistical learning

$\mathcal{Y}, \Delta$

- The output space might not be a linear space and can be continuous.
- Structure encoded by the loss function.

Beyond finite, discrete spaces to include continuous output spaces, e.g.
- Manifold regression [14],
- prediction of probability distributions [15].
Inner SELF (risk)

\[ \int d\rho(y|x) \Delta(f(x), y) = \int d\rho(y|x) \langle \Psi(y), \Phi(y') \rangle = \left\langle \int d\rho(y|x) \Psi(y), \Phi(y') \right\rangle_{g_\ast(x)} \]
Inner SELF (risk)

\[ \int d\rho(y|x) \Delta(f(x), y) = \int d\rho(y|x) \langle \Psi(y), \Phi(y') \rangle = \left\langle \int d\rho(y|x) \Psi(y), \Phi(y') \right\rangle \]

Lemma (Ciliberto, Rudi, R. '17)

\[ f_*(x) = \arg\min_{y \in \mathcal{Y}} \langle g_*(x), \Phi(y) \rangle \]

\[ g_* = \int d\rho(y|x) \Psi(y) = \arg\min_{g \in \mathcal{H}^X} \int d\rho(x, y) \|g(x) - \Psi(y)\|^2 \]
Inner risk minimization (IRM)

\[
\hat{f}(x) = \arg\min_{y \in \mathcal{Y}} \langle \hat{g}(x), \Phi(y) \rangle
\]

\[
\hat{g} = \arg\min_{g \in \mathcal{G} \subset \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \|g(x_i) - \Psi(y_i)\|^2
\]
IRM: a general surrogate approach

- encode $\Psi : \mathcal{Y} \rightarrow \mathcal{H}$
- learn $(x_i, \Psi(y_i))_{i=1}^{n} \mapsto \hat{g}$
- decode $\Psi^* : \mathcal{H} \rightarrow \mathcal{Y}$

$$\Psi^*(h) = \arg\min_{y \in \mathcal{Y}} \langle h, \Phi(y) \rangle, \quad h \in \mathcal{H}.$$
Some questions

- A minimization over $\mathcal{Y}$ instead of $\mathcal{Y}^\chi$: what we gained?

- Does a SELF exist?
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Solving IRM with linear estimators

\[ \hat{f}(x) = \arg\min_{y \in \mathcal{Y}} \langle \hat{g}(x), \Phi(y) \rangle, \quad \hat{g} = \arg\min_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \|g(x_i) - \Psi(y_i)\|^2. \]
Solving IRM with linear estimators

\[ \hat{f}(x) = \arg\min_{y \in \mathcal{Y}} \langle \hat{g}(x), \Phi(y) \rangle, \quad \hat{g} = \arg\min_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \| g(x_i) - \Psi(y_i) \|^2. \]

Lemma (Ciliberto, Rudi, R. ’17)

If \( g(x) = W x \), then

\[ W = (\hat{X}^\top \hat{X})^{-1} \hat{X}^\top \hat{Y}, \quad \hat{X} \in \mathbb{R}^{n \times d}, \quad \hat{Y} \in \mathcal{H}^{n} \]

and

\[ \hat{g}(x) = \sum_{i=1}^{n} \alpha_i(x) \Psi(y_i), \quad \alpha(x) = (\hat{X} \hat{X}^\top)^{-1} \hat{X} x \in \mathbb{R}^{n} \]
Implicit IRM for linear estimators

\[ \hat{f}(x) = \arg\min_{y \in \mathcal{Y}} \langle \hat{g}(x), \Phi(y) \rangle, \quad \hat{g} = \arg\min_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \| g(x_i) - \Psi(y_i) \|^2. \]

Lemma (Ciliberto, Rudi, R. ’17)

If

\[ \hat{g}(x) = \sum_{i=1}^{n} \alpha_i(x) \Psi(y_i), \]

then

\[ \hat{f}(x) = \arg\min_{y \in \mathcal{Y}} \sum_{i=1}^{n} \alpha_i(x) \Delta(y_i, y) \]
Other linear estimators

\[ \hat{g}(x) = \sum_{i=1}^{n} \alpha_i(x) \Psi(y_i), \]

- Kernel methods \( g(x) = W \gamma(x), \) where \( \gamma : \mathcal{X} \to (\mathcal{H}_\Gamma, \langle \cdot, \cdot \rangle_\Gamma). \)
- Local kernel estimators.
- Spectral filters.
- Sketching/random features/Nyström.
Computations: no free lunch

Training

\[ \hat{g} = \arg\min_{g \in G} \frac{1}{n} \sum_{i=1}^{n} \|g(x_i) - \Psi(y_i)\|^2. \]

Computing \((\alpha_i(x))_i\) depends only on the inputs and is efficient.

Prediction

\[ \hat{f}(x) = \arg\min_{y \in Y} \sum_{i=1}^{n} \alpha_i(x) \Delta(y_i, y). \]

Requires problem specific decoding and can be hard.
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Consistency and excess risk bounds

**Problem** Solve

\[
\min_{f \in \mathcal{Y}} R(f), \quad R(f) = \int d\rho(x, y) \Delta(f(x), y)
\]

given \((x_i, y_i)_{i=1}^n\) i.i.d. samples of \(\rho\).

**Excess risk** Convergence and rates on

\[
R(\hat{f}) - R(f^*)
\]
A relaxation error analysis

Let

\[ L(g) = \int d\rho(x, y) \| g(x) - \Psi(y) \|^2 \]

Theorem (Ciliberto, Rudi, R. ’17)

The following hold:

- **Fisher consistency**
  \[ f_\star(x) = \Psi_\star g_\star(x). \text{ a.s.} \]

- **Comparison inequality, for all } g \text{ and } f(x) = \Psi_\star g(x) \text{ a.s.}
  \[ R(f) - R(f_\star) \leq c_\Delta \sqrt{L(g) - L(g_\star)} \]

where

\[ c_\Delta = \sup_{y \in Y} \| \Psi(y) \| \]
Consistency and rates for IRM-KRR

Let \( \hat{g}_\lambda(x) = \hat{W}_\lambda \gamma(x) \) with

\[
\hat{W}_\lambda = \arg\min_{W \in \mathcal{L}_2(\mathcal{H}_\Gamma, \mathcal{H})} \frac{1}{n} \sum_{i=1}^{n} \|W x_i - \Psi(y_i)\|^2 + \lambda \|W\|_2^2.
\]

Theorem (Ciliberto, Rudi, R. '17)

Let \( \kappa_\gamma = \sup_{x \in \mathcal{X}} \|\gamma(x)\| \). Assume \( \exists W_* \in \mathcal{L}_2(\mathcal{H}_\Gamma, \mathcal{H}) \) such that \( g_*(x) = W_* x \). If \( \lambda_n = O(1/\sqrt{n}) \), then with probability at least \( 1 - 8e^{-\tau} \)

\[
\sqrt{L(\hat{g}) - L(g_*)} \leq 24 \kappa_\gamma \left( 1 + \|W\|_2 \right) \tau^2 n^{-1/4}.
\]

and for \( \hat{f}(x) = \Psi^* \hat{g}_\lambda(x) \) a.s.

\[
R(\hat{f}) - R(f_*) \leq 24 \kappa_\gamma c_\Delta (1 + \|W\|_2) \tau^2 n^{-1/4}.
\]
Remarks

- This is the first result establishing consistency and rates for structured prediction, see [13] for similar efforts.

- The bound on $L(\hat{g}) - L(g_\star)$ extend results in [17] under weaker assumptions.

- The constant $c_\Delta$ is problem dependent. Finding a general estimate is an open problem [18].
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Ranking

<table>
<thead>
<tr>
<th>Method</th>
<th>Rank Loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear [8]</td>
<td>0.430 ± 0.004</td>
</tr>
<tr>
<td>Hinge [19]</td>
<td>0.432 ± 0.008</td>
</tr>
<tr>
<td>Logistic [20]</td>
<td>0.432 ± 0.012</td>
</tr>
<tr>
<td>SVM Struct [9]</td>
<td>0.451 ± 0.008</td>
</tr>
<tr>
<td>IRM-KRR</td>
<td>0.396 ± 0.003</td>
</tr>
</tbody>
</table>

Ranking movies in the MovieLens dataset [21] (ratings (from 1 to 5) of 1682 movies by 943 users). The goal is predict preferences of a given user, i.e. an ordering of the 1682 movies, according to the user’s partial ratings. We use the loss [8]

\[ \Delta_{rank}(y, y') = \frac{1}{2} \sum_{i,j=1}^{M} \gamma(y'_{ij}) (1 - \text{sign}(y_i - y_j)), \]
Average absolute error (in degrees) for the manifold structured estimator (SP), the manifold regression (MR) approach in [14] and the KRLS baseline. (Right) Fingerprint reconstruction of a single image where the structured predictor achieves 15.7 of average error while KRLS 25.3. The loss is the geodesic on $S$

$$\Delta_S(z, y) = \arccos (\langle z, y \rangle)^2$$
Summing up

- First consistent algorithmic framework for StructML.
- A general surrogate approach.
- TBD: decoding computations+ beyond linear estimators.

Openings

Multiple openings for post-docs/PhD positions!

→ Launching: Machine Learning Genova Center!
Related papers

Bakir Gökhan, Thomas Hofmann, Bernhard Schölkopf, Alexander J. Smola, Ben Taskar, and S.V.N Vishwanathan.
Predicting structured data.

Karteek Alahari, Pushmeet Kohli, and Philip HS Torr.
Reduce, reuse & recycle: Efficiently solving multi-label mrfs.

Andrej Karpathy and Li Fei-Fei.
Deep visual-semantic alignments for generating image descriptions.

Lalit Bahl, Peter Brown, Peter De Souza, and Robert Mercer.
Maximum mutual information estimation of hidden markov model parameters for speech recognition.

Charles Sutton, Andrew McCallum, et al.
An introduction to conditional random fields.

Thorsten Joachims, Thomas Hofmann, Yisong Yue, and Chun-Nam Yu.
Predicting structured objects with support vector machines.

Fabian Pedregosa, Francis Bach, and Alexandre Gramfort.
On the consistency of ordinal regression methods.

John C Duchi, Lester W Mackey, and Michael I Jordan.
On the consistency of ranking algorithms.
In Proceedings of the 27th International Conference on Machine Learning (ICML-10),

Ioannis Tsochantaridis, Thorsten Joachims, Thomas Hofmann, and Yasemin Altun.
Large margin methods for structured and interdependent output variables.

Sebastian Nowozin, Christoph H Lampert, et al.
Structured learning and prediction in computer vision.
Peter L Bartlett, Michael I Jordan, and Jon D McAuliffe.  
Convexity, classification, and risk bounds.  

Youssef Mroueh, Tomaso Poggio, Lorenzo Rosasco, and Jean-Jacques Slotine.  
Multiclass learning with simplex coding.  

Anton Osokin, Francis Bach, and Simon Lacoste-Julien.  
On structured prediction theory with calibrated convex surrogate losses.  

Florian Steinke, Matthias Hein, and Bernhard Schölkopf.  
Nonparametric regression between general riemannian manifolds.  

Charlie Frogner, Chiyuan Zhang, Hossein Mobahi, Mauricio Araya, and Tomaso A Poggio.  
Learning with a wasserstein loss.  

Jason Weston, Olivier Chapelle, Vladimir Vapnik, André Elisseeff, and Bernhard Schölkopf.  
Kernel dependency estimation.
Andrea Caponnetto and Ernesto De Vito.  
Optimal rates for the regularized least-squares algorithm.  

Alex Nowak-Vila, Francis Bach, and Alessandro Rudi.  
Sharp analysis of learning with discrete losses.  

Ralf Herbrich, Thore Graepel, and Klaus Obermayer.  
Large margin rank boundaries for ordinal regression.  

Ofer Dekel, Yoram Singer, and Christopher D Manning.  
Log-linear models for label ranking.  

F Maxwell Harper and Joseph A Konstan.  
The movielens datasets: History and context.  