# Feature-aware Label Space Dimension Reduction for Multi-label Classification

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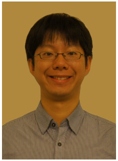
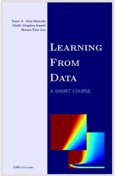
*first part: with Farbound Tai, in Neural Computation 2012*
*second part: with Yao-Nan Chen, in NIPS 2012*

# A Short Introduction

## Hsuan-Tien Lin



- Associate Professor, CSIE, National Taiwan University
- Secretary General, TAAI
- Co-author of the introductory ML textbook "*Learning from Data: A Short Course*" (Amazon ML best seller!)
- Leader of the Computational Learning Laboratory

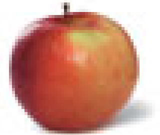



### goal: make machine learning **more realistic**

- multi-class cost-sensitive classification: in ICML '10, BIBM '11, KDD '12, etc.
- online/active learning: in ACML '11, ICML '12, ACML '12
- video search: in CVPR '11
- multi-label classification: in ACML '11, NIPS '12, etc.
- large-scale data mining (w/ Profs. S.-D. Lin & C.-J. Lin & students): third place of KDDCup '09, champions of '10, '11 ($\times 2$), '12

# Which Fruit?

**?**



apple

orange

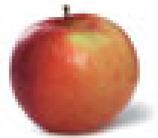
strawberry

kiwi

multi-class classification:
classify input (picture) to **one category** (label)

# Which Fruits?

**?**: {orange, strawberry, kiwi}



apple

orange

strawberry

kiwi

multi-label classification:
classify input to **multiple (or no)** categories

# Powerset: Multi-label Classification via Multi-class

**Multi-class w/ $L = 4$ classes**

4 possible outcomes

{a, o, s, k}

**Multi-label w/ $L = 4$ classes**

$2^4 = 16$ **possible outcomes**

$2^{\{\text{a, o, s, k}\}}$

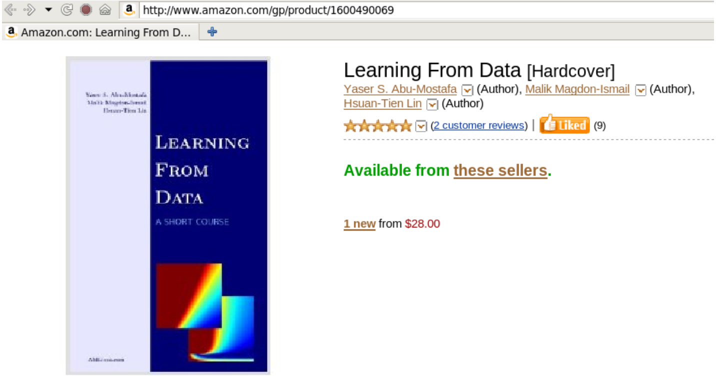
$\Updownarrow$

{ $\phi$, a, o, s, k, ao, as, ak, os, ok, sk, aos, aok, ask, osk, aosk }

- **Powerset** approach: transformation to multi-class classification
- difficulties for large $L$:
  - **computation** (super-large $2^L$)
    —hard to construct classifier
  - **sparsity** (no example for some of $2^L$)
    —hard to discover hidden combination

**Powerset**: feasible only for small $L$ with enough examples for every combination

# What Tags?




**?**: {machine learning, ~~data structure~~, data mining, ~~object oriented programming~~, artificial intelligence, ~~compiler~~, ~~architecture~~, ~~chemistry~~, textbook, ~~children book~~, ~~. . . etc.~~ }

another **multi-label** classification problem:
**tagging** input to multiple categories

# Binary Relevance: Multi-label Classification via Yes/No

**Binary Classification**

{yes, no}

**Multi-label w/ $L$ classes: $L$ yes/no questions**

machine learning (Y), data structure (N), data mining (Y), OOP (N), AI (Y), compiler (N), architecture (N), chemistry (N), textbook (Y), children book (N), *etc.*

- **Binary Relevance** approach:
  transformation to **multiple isolated binary classification**
- disadvantages:
  - **isolation**—hidden relations not exploited (e.g. ML and DM highly correlated, ML subset of AI, textbook & children book disjoint)
  - **unbalanced**—few yes, many no

**Binary Relevance**: simple (& good) benchmark with known disadvantages

# Multi-label Classification Setup

## Given

$N$ examples (input $\mathbf{x}_n$, label-set $\mathcal{Y}_n$) $\in \mathcal{X} \times 2^{\{1,2,\cdots L\}}$

- `fruits`: $\mathcal{X} =$ encoding(pictures), $\mathcal{Y}_n \subseteq \{1, 2, \cdots, 4\}$
- `tags`: $\mathcal{X} =$ encoding(merchandise), $\mathcal{Y}_n \subseteq \{1, 2, \cdots, L\}$

## Goal

a multi-label classifier $g(\mathbf{x})$ that **closely predicts** the label-set $\mathcal{Y}$ associated with some **unseen** inputs $\mathbf{x}$ (by exploiting hidden relations/combinations between labels)

- **Hamming loss**: averaged symmetric difference $\frac{1}{L}|g(\mathbf{x}) \triangle \mathcal{Y}|$

**multi-label classification: hot and important**

# From Label-set to Coding View

| | label set | apple | orange | strawberry | binary code |
|---|---|---|---|---|---|
|  | $\mathcal{Y}_1 = \{\text{o}\}$ | 0 (N) | 1 (Y) | 0 (N) | $\mathbf{y}_1 = [0, 1, 0]$ |
|  | $\mathcal{Y}_2 = \{\text{a, o}\}$ | 1 (Y) | 1 (Y) | 0 (N) | $\mathbf{y}_2 = [1, 1, 0]$ |
|  | $\mathcal{Y}_3 = \{\text{a, s}\}$ | 1 (Y) | 0 (N) | 1 (Y) | $\mathbf{y}_3 = [1, 0, 1]$ |
|  | $\mathcal{Y}_4 = \{\text{o}\}$ | 0 (N) | 1 (Y) | 0 (N) | $\mathbf{y}_4 = [0, 1, 0]$ |
|  | $\mathcal{Y}_5 = \{\}$ | 0 (N) | 0 (N) | 0 (N) | $\mathbf{y}_5 = [0, 0, 0]$ |

subset $\mathcal{Y}$ of $2^{\{1,2,\cdots,L\}}$ $\Leftrightarrow$ **length-$L$ binary code $\mathbf{y}$**

# Existing Approach: Compressive Sensing

## General Compressive Sensing

sparse (many 0) binary vectors $\mathbf{y} \in \{0, 1\}^L$ can be **robustly compressed** by projecting to $M \ll L$ basis vectors $\{\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_M\}$

## Compressive Sensing for Multi-label Classification (Hsu et al., 2009)

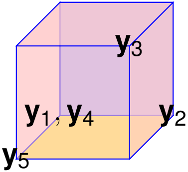
1. **compress**: transform $\{(\mathbf{x}_n, \mathbf{y}_n)\}$ to $\{(\mathbf{x}_n, \mathbf{c}_n)\}$ by $\mathbf{c}_n = \mathbf{P}\mathbf{y}_n$ with some $M$ by $L$ random matrix $\mathbf{P} = [\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_M]^T$
2. **learn**: get regression function $\mathbf{r}(\mathbf{x})$ from $\mathbf{x}_n$ to $\mathbf{c}_n$
3. **decode**: $g(\mathbf{x})$ = find closest sparse binary vector to $\mathbf{P}^T\mathbf{r}(\mathbf{x})$

**Compressive Sensing**:

- efficient in training: random projection w/ $M \ll L$
- inefficient in testing: time-consuming decoding

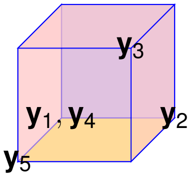
# From Coding View to Geometric View

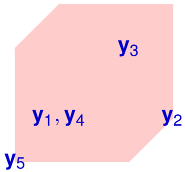
| | label set | binary code |
|---|---|---|
|  | $\mathcal{Y}_1 = \{o\}$ | $\mathbf{y}_1 = [0, 1, 0]$ |
|  | $\mathcal{Y}_2 = \{a, o\}$ | $\mathbf{y}_2 = [1, 1, 0]$ |
|  | $\mathcal{Y}_3 = \{a, s\}$ | $\mathbf{y}_3 = [1, 0, 1]$ |
|  | $\mathcal{Y}_4 = \{o\}$ | $\mathbf{y}_4 = [0, 1, 0]$ |
|  | $\mathcal{Y}_5 = \{\}$ | $\mathbf{y}_5 = [0, 0, 0]$ |




length-$L$ binary code $\Leftrightarrow$ **vertex of hypercube** $\{0, 1\}^L$

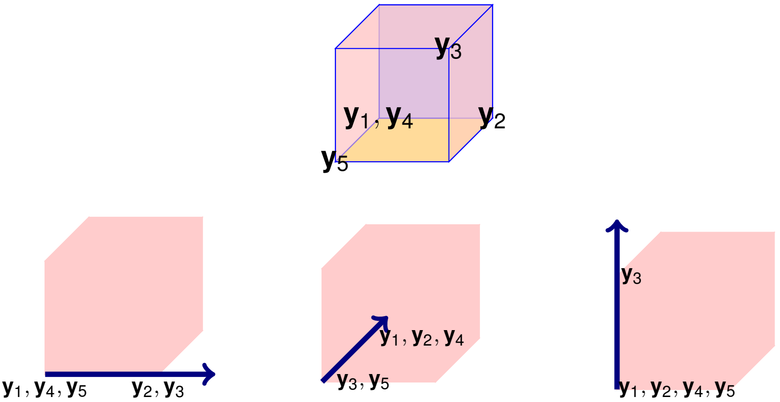
# Geometric Interpretation of Powerset



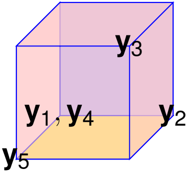



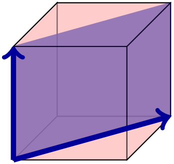

Powerset: directly classify to the **vertices** of hypercube

# Geometric Interpretation of Binary Relevance




Binary Relevance: project to the **natural axes** & classify



Compressive Sensing:

- project to **random flat** (linear subspace)
- learn "on" the flat; decode to closest sparse vertex

other (better) flat? other (faster) decoding?

# Our Contributions

**Two Novel Approaches for Label Space Dimension Reduction**

- algorithmic: scheme for fast decoding
- theoretical: justification for best projection, one feature-unaware and the other feature-aware
- practical: significantly better performance than compressive sensing (& binary relevance)

will now introduce the key ideas behind the approaches

# Faster Decoding: Round-based

## Compressive Sensing Revisited

- **decode**: $g(\mathbf{x})$ = sparse binary vector that **P**-projects closest to $\mathbf{r}(\mathbf{x})$

For any given "prediction on subspace" $\mathbf{r}(\mathbf{x})$,

- find sparse binary vector that **P**-projects closest to $\mathbf{r}(\mathbf{x})$: slow —optimization of $\ell_1$-regularized objective
- find any binary vector that **P**-projects closest to $\mathbf{r}(\mathbf{x})$: fast

$$g(\mathbf{x}) = \text{round}(\mathbf{P}^T \mathbf{r}(\mathbf{x})) \text{ for orthogonal } \mathbf{P}$$

round-based decoding: simple & faster alternative

# Better Projection: Principal Directions

## Compressive Sensing Revisited

- **compress**: transform $\{(\mathbf{x}_n, \mathbf{y}_n)\}$ to $\{(\mathbf{x}_n, \mathbf{c}_n)\}$ by $\mathbf{c}_n = \mathbf{P}\mathbf{y}_n$ with some $M$ by $L$ random matrix $\mathbf{P}$

- random projection: arbitrary directions
- best projection: principal directions

principal directions: best approximation to desired output $\mathbf{y}_n$ during dimension reduction (**why?**)

# Novel Theoretical Guarantee

Linear Transform + Learn + Round-based Decoding

**Theorem (Tai and Lin, 2012)**

*If* $g(\mathbf{x}) = \mathit{round}(\mathbf{P}^T\mathbf{r}(\mathbf{x}))$ *(& $\mathbf{p}_m$ orthogonal to each other),*

$$\underbrace{\frac{1}{L}|g(\mathbf{x}) \triangle \mathcal{Y}|}_{\text{Hamming loss}} \leq \mathit{const} \cdot \left( \underbrace{\|\mathbf{r}(\mathbf{x}) - \overbrace{\mathbf{P}\mathbf{y}}^{\mathbf{c}}\|^2}_{\text{learn}} + \underbrace{\|\mathbf{y} - \mathbf{P}^T\overbrace{\mathbf{P}\mathbf{y}}^{\mathbf{c}}\|^2}_{\text{compress}} \right)$$

- $\|\mathbf{r}(\mathbf{x}) - \mathbf{c}\|^2$: prediction error from input to codeword
- $\|\mathbf{y} - \mathbf{P}^T\mathbf{c}\|^2$: encoding error from desired output to codeword

principal directions: best approximation to desired output $\mathbf{y}_n$ during dimension reduction (**indeed**)

# Proposed Approach: Principal Label Space Transform

## From Compressive Sensing to PLST

1. **compress**: transform $\{(\mathbf{x}_n, \mathbf{y}_n)\}$ to $\{(\mathbf{x}_n, \mathbf{c}_n)\}$ by $\mathbf{c}_n = \mathbf{P}\mathbf{y}_n$ with the $M$ by $L$ principal matrix $\mathbf{P}$
2. **learn**: get regression function $\mathbf{r}(\mathbf{x})$ from $\mathbf{x}_n$ to $\mathbf{c}_n$
3. **decode**: $g(\mathbf{x}) = \text{round}(\mathbf{P}^T\mathbf{r}(\mathbf{x}))$

- principal directions: via Principal Component Analysis on $\{\mathbf{y}_n\}_{n=1}^{N}$ —BTW, improvements when shifting $\mathbf{y}_n$ by its estimated mean
- physical meaning behind $\mathbf{p}_m$: key (linear) label correlations

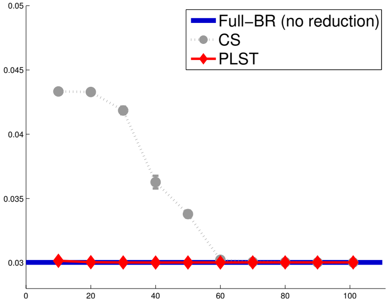
PLST: improving CS by projecting to **key correlations**

# PLST vs. CS

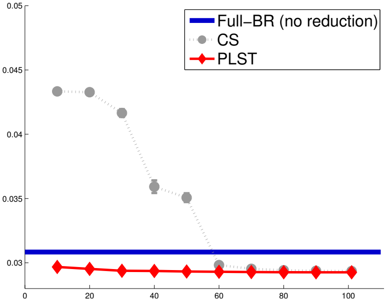
| | PLST | CS |
|---|---|---|
| Compress | projection through SVD (principal directions) | random basis projection (random directions) |
| Learn | multi-output regression | |
| Decode | round-based (fast) | sparsity-based (slower) |

**practical performance?**

# Hamming Loss Comparison: Full-BR, PLST & CS




mediamill (Linear Regression)




mediamill (Decision Tree)

- PLST better than Full-BR: fewer dimensions, similar (or **better**) performance
- PLST better than CS: faster, **better** performance
- similar findings across **data sets** and **regression algorithms**

# Theoretical Guarantee of PLST Revisited

Linear Transform + Learn + Round-based Decoding

**Theorem (Tai and Lin, 2012)**

If $g(\mathbf{x}) = \mathit{round}(\mathbf{P}^T \mathbf{r}(\mathbf{x}))$,

$$\underbrace{\frac{1}{L}|g(\mathbf{x}) \triangle \mathcal{Y}|}_{\text{Hamming loss}} \le \mathit{const} \cdot \left( \underbrace{\|\mathbf{r}(\mathbf{x}) - \overbrace{\mathbf{Py}}^{\mathbf{c}}\|^2}_{\text{learn}} + \underbrace{\|\mathbf{y} - \mathbf{P}^T \overbrace{\mathbf{Py}}^{\mathbf{c}}\|^2}_{\text{compress}} \right)$$

- $\|\mathbf{y} - \mathbf{P}^T\mathbf{c}\|^2$: encoding error, minimized during encoding
- $\|\mathbf{r}(\mathbf{x}) - \mathbf{c}\|^2$: prediction error, minimized during learning
- but good encoding may not be easy to learn; vice versa

PLST: minimize two errors separately (**sub-optimal**)
(can we do even better by minimizing **jointly**?)

# The In-Sample Optimization Problem

$$\min_{\mathbf{r},\mathbf{P}} \left( \underbrace{\|\mathbf{r}(\mathbf{X}) - \mathbf{P}\mathbf{Y}\|^2}_{\text{learn}} + \underbrace{\|\mathbf{Y} - \mathbf{P}^T\mathbf{P}\mathbf{Y}\|^2}_{\text{compress}} \right)$$

- start from a well-known tool, linear regression, as $\mathbf{r}$

$$\mathbf{r}(\mathbf{X}) = \mathbf{X}\mathbf{W}$$

- for fixed $\mathbf{P}$: a closed-form solution for learn is

$$\mathbf{W}^* = \mathbf{X}^\dagger\mathbf{P}\mathbf{Y}$$

- substitute $\mathbf{W}^*$ to objective function, then ...

optimal $\mathbf{P}$:

| | |
|---|---|
| for learn | top eigenvectors of $\mathbf{Y}^T(\mathbf{I} - \mathbf{X}\mathbf{X}^\dagger)\mathbf{Y}$ |
| for compress | top eigenvectors of $\mathbf{Y}^T\mathbf{Y}$ |
| for both | top eigenvectors of $\mathbf{Y}^T\mathbf{X}\mathbf{X}^\dagger\mathbf{Y}$ |

# Proposed Approach: Conditional Principal Label Space Transform

## From PLST to CPLST

1. **compress**: transform $\{(\mathbf{x}_n, \mathbf{y}_n)\}$ to $\{(\mathbf{x}_n, \mathbf{c}_n)\}$ by $\mathbf{c}_n = \mathbf{P}\mathbf{y}_n$ with the $M$ by $L$ conditional principal matrix $\mathbf{P}$
2. **learn**: get regression function $\mathbf{r}(\mathbf{x})$ from $\mathbf{x}_n$ to $\mathbf{c}_n$, ideally using linear regression
3. **decode**: $g(\mathbf{x}) = \text{round}(\mathbf{P}^T\mathbf{r}(\mathbf{x}))$

- conditional principal directions: top eigenvectors of $\mathbf{Y}^T\mathbf{X}\mathbf{X}^{\dagger}\mathbf{Y}$
- physical meaning behind $\mathbf{p}_m$: key (linear) label correlations that are "easy to learn" subject to the features (feature-aware)

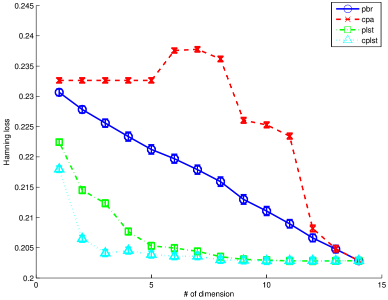
CPLST: **feature-aware** label space dimension reduction
—can also pair with **kernel regression (non-linear)**

# CPLST vs. PLST

| | CPLST | PLST |
|---|---|---|
| Compress | Linear/Kernel Regression + SVD<br>(conditional principal directions) | SVD<br>(principal directions) |
| Learn | multi-output regression | |
| Decode | round-based<br>(fast) | |

**practical performance?**

# Hamming Loss Comparison: PLST & CPLST




yeast (Linear Regression)

- CPLST better than PLST: better performance across all dimensions
- similar findings across **data sets** and **regression algorithms** (even decision trees)

# Conclusion

## PLST

- transformation to **multi-output regression**
- project to **principal directions** and capture key correlations
- efficient learning (after **label space dimension reduction**)
- efficient decoding (**round**)
- sound theoretical guarantee
- **good practical performance** (better than CS & BR)

## CPLST

- project to **conditional** (feature-aware) principal directions and capture key **learnable** correlations
- can be **kernelized** for exploiting feature power
- sound theoretical guarantee (via PLST)
- **even better practical performance** (than PLST)

Thank you! Questions?