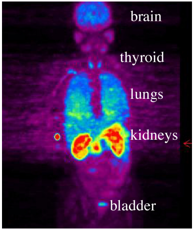
The pyramid quantized Weisfeiler-Lehman graph representation

Katerina Gkirtzou & Matthew Blaschko

January 8, 2014

Medical Imaging

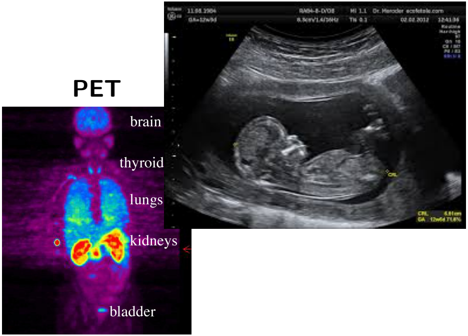
PET



Medical Imaging

Ultrasound

PET



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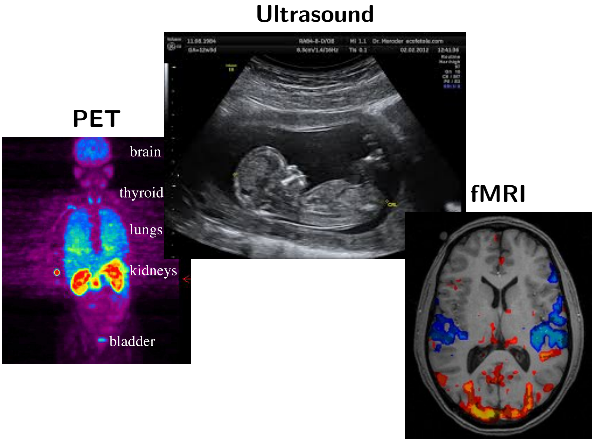

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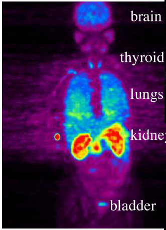
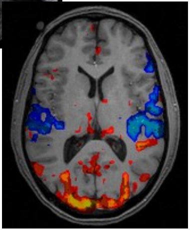
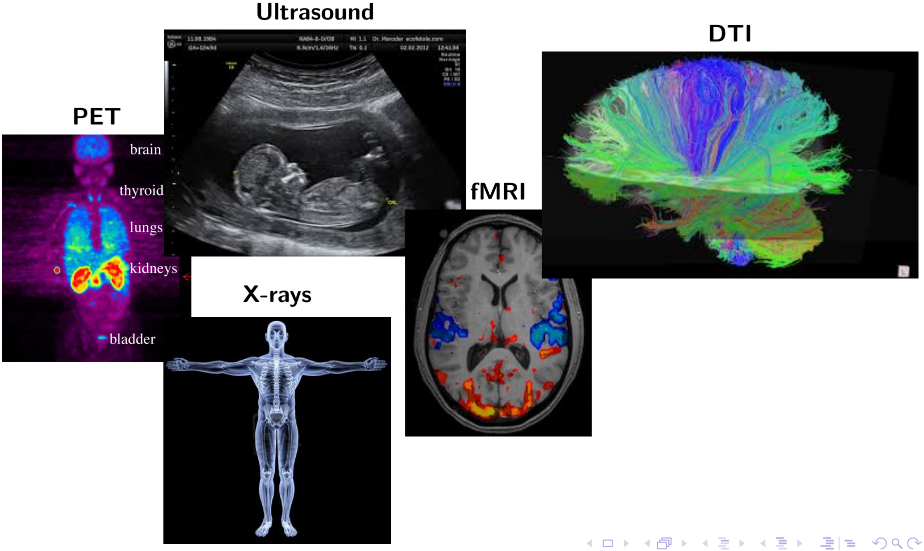


fMRI

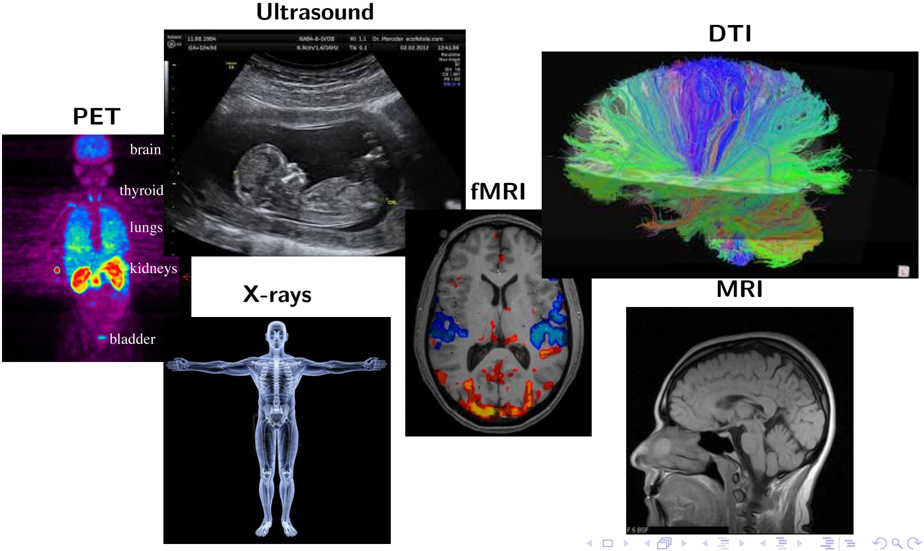


X-rays

Medical Imaging

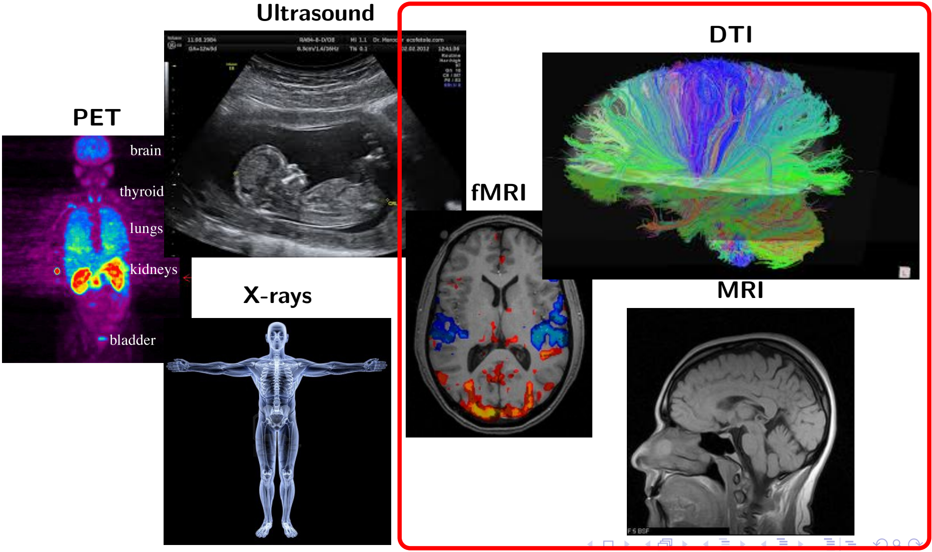


Medical Imaging



Medical Imaging

Image Classification



Medical image classification

Given a set of n paired observations $\{(\mathbb{I}_i, y_i)\}_{1 \leq i \leq n}$ where

- $\mathbb{I}_i$ is an medical image and
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the goal is to learn a *classification function* f.

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1. The representation of $\phi(\mathbb{I})$.
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2. Supervised statistical learning framework

$$\arg\min_{f \in \mathcal{F}} \lambda\Omega(f) + \overbrace{\frac{1}{n}\sum_{i=1}^{n} \mathbb{L}(f(\phi(\mathbb{I}_i)), y_i)}^{\text{Empirical Risk}}$$

where $\mathbb{L}$ is the *loss function* and $\lambda\Omega(f)$ is the regularization term.

Table of Content

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What is a graph and why is it interesting?

Definition

A *labeled graph* G is defined as a triplet $(V, E, \mathcal{L})$, where V is the *vertex set* and $E \subseteq V \times V$ is the *edge set* which represents a binary relation on V and $\mathcal{L} : X \mapsto \Sigma$ is a function assigning a label from an alphabet Σ to each element of the set X, which can be either V, E or $V \cup E$.

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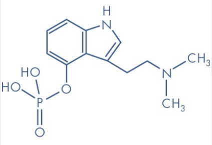

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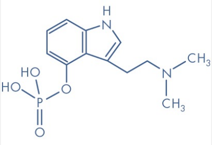

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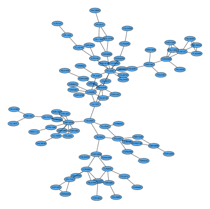

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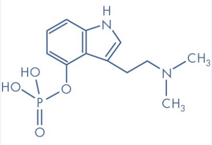

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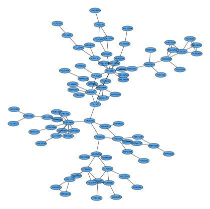

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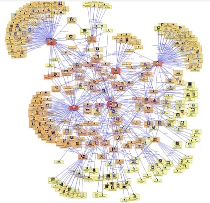

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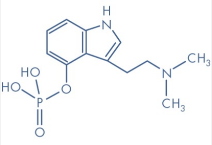

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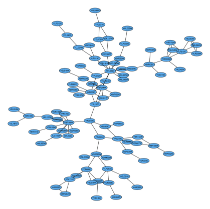

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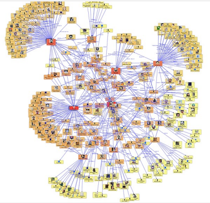

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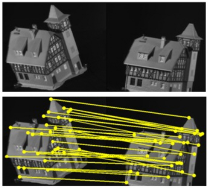

Computer Vision

Graph Comparison Problem

Definition

Given a set $\mathcal{G}$ of graphs, the problem of graph comparison is defined as a function

$$k : \mathcal{G} \times \mathcal{G} \mapsto \mathbb{R}$$

such that $k(G, G')$ for $G, G' \in \mathcal{G}$ quantifies the similarity of G and G'.

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1st Approach

- Graph Isomorphism
- Subgraph Isomorphism
- Largest common subgraph

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1st Approach

- Graph Isomorphism - No efficient algorithm is known
- Subgraph Isomorphism - Proven to be NP-complete
- Largest common subgraph - Proven to be NP-hard

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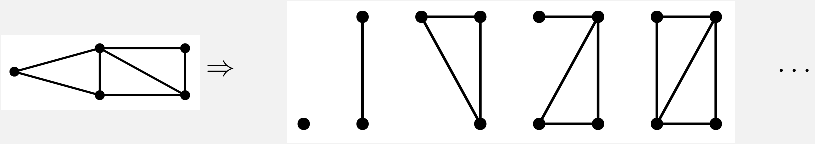
2nd Approach - R-convolution Kernels



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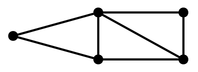
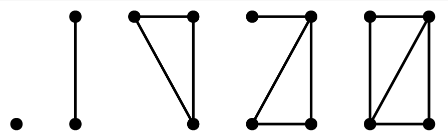


$\Rightarrow$



$\cdots$

Calculating all subgraphs is at least as hard as deciding whether two graphs are isomorphic [Gärtner 03]

Graph kernels

	Algorithm	Complexity[1]	Unlabeled	Discrete	Continuous	Vector
Walks	[Gärtner 03]	$\mathcal{O}(n^2 v^6)$	✓	✓	✓	✓
	[Mahé 04]		✓	✓		
	[Vishwanathan 10]	$\mathcal{O}(n^2 v^3)$	✓	✓	✓	✓
Paths	[Borgwardt 05]	$\mathcal{O}(n^2 v^4)$	✓	✓	✓	✓
	[Ralaivola 05]		✓	✓		
Graphlets	[Horváth 04]		✓	✓		
	[Shervashidze 09]	$\mathcal{O}(vd^{k-1})$	✓			
	[Costa 10]		✓	✓		
Subtree Patterns	[Ramon 03]	$\mathcal{O}(n^2 v^2 h 4^d)$	✓	✓		
	[Bach 08]		✓	✓		
	[Mahé 09]		✓	✓		
	[Shervashidze 11]	$\mathcal{O}(nhe + n^2 hv)$	✓	✓		

---

[1] where n is the number of graphs, v is the maximal number of nodes, e is the maximal number of edges, h is the height of subtree patterns, d is the maximum degree and k is the size of graphlets.

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Overview of the WLpyramid

Given a set $\mathcal{G} = \{G_i = (V_i, E_i, \mathcal{L}_i)\}_{1 \leq i \leq n}$ where $\mathcal{L}_i : V_i \mapsto \mathbb{R}^d$

1. A pyramid quantization of the label space.
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3. Produce subtree features with Weisfeiler-Lehman algorithm.
4. Learning the combination of the subtree features.

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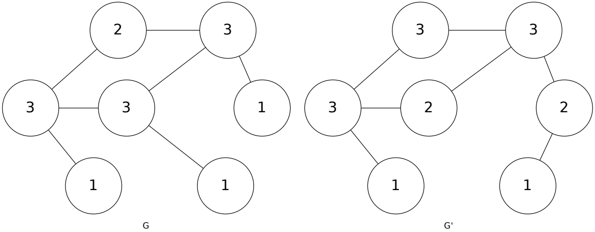
Why Weisfeiler-Lehman?

1. Computational time $\mathcal{O}(nhe)$
   - n the number of graphs
   - e the maximal number of edges and and
   - h the height subtree features.
2. Competitive accuracy in several classification benchmark data sets [Shervashidze 11].

The Weisfeiler-Lehman test of isomorphism [Weisfeiler 68]

Given labeled graphs G and G'



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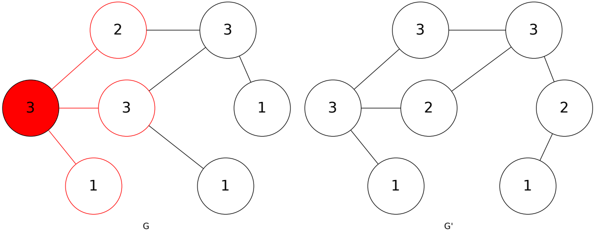
Multi-label determination of G and G'



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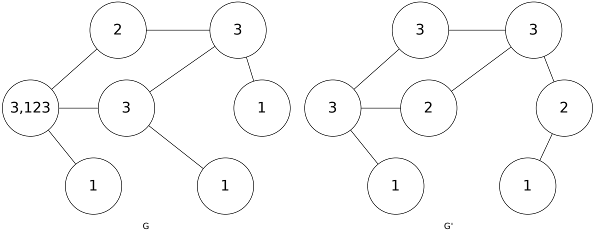

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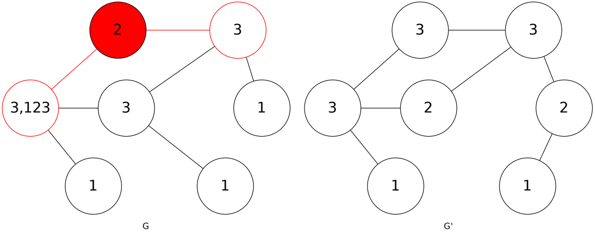

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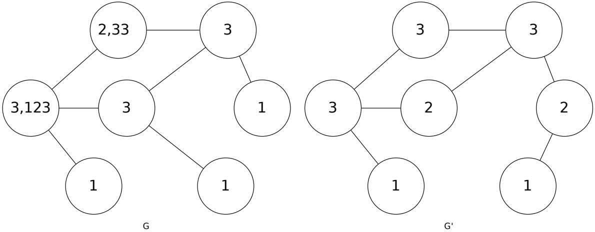

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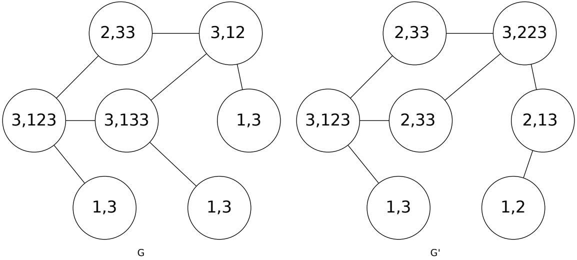

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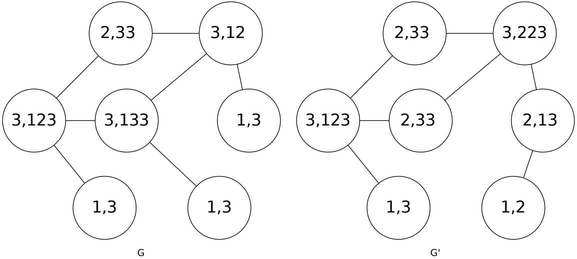

Label compression via hashing

1,2 ⟶ 4

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2,13 ⟶ 6

2,33 ⟶ 7

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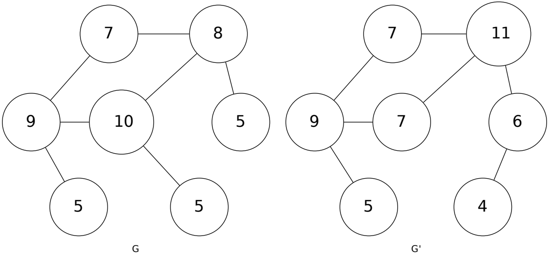
Relabeling graphs G and G'



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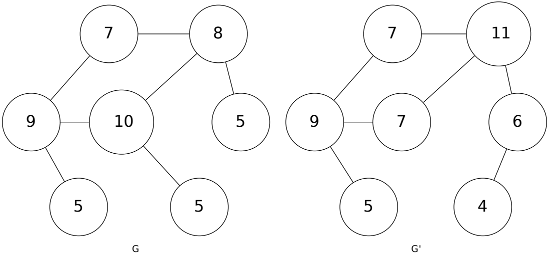

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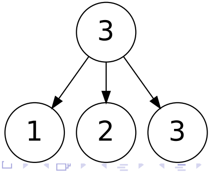
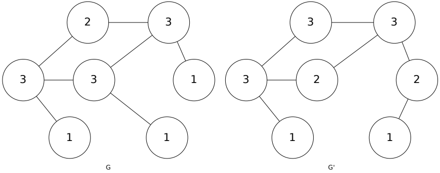
Subtree Pattern of Compressed label 9



Weisfeiler-Lehman subtree features

Subtree patterns of depth 0.



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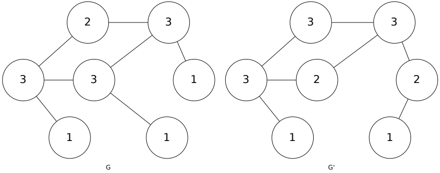
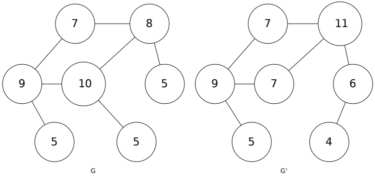


Subtree patterns of depth 1.



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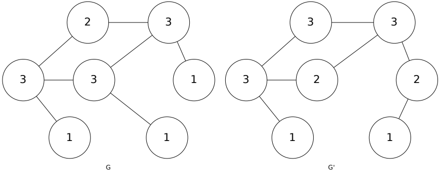

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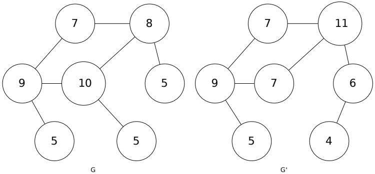
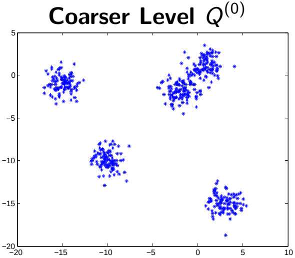


$$\begin{array}{rcl}
\text{Labels } \{\Sigma_0, \Sigma_1\} & = & \{\overbrace{1,\ \ 2,\ \ 3,}^{\text{Original node labels } \Sigma_0}\ \ \overbrace{4,\ \ 5,\ \ 6,\ \ 7,\ \ 8,\ \ 9,\ \ 10,\ \ 11}^{\text{Compressed node labels } \Sigma_1}\} \\
\phi_{(1)}(G) & = & (3,\ \ 1,\ \ 3,\ \ 0,\ \ 3,\ \ 0,\ \ 1,\ \ 1,\ \ 1,\ \ 1,\ \ 0) \\
\phi_{(1)}(G') & = & (2,\ \ 2,\ \ 3,\ \ 1,\ \ 1,\ \ 1,\ \ 2,\ \ 0,\ \ 1,\ \ 0,\ \ 1)
\end{array}$$

$\phi_{(h)}(G)$ are histograms of occurences of the subtree patterns up to depth h in graph G.

The pyramid quantization strategy

Given a set $\mathcal{G} = \{G_i = (V_i, E_i, \mathcal{L}_i)\}_{1 \leq i \leq n}$ where $\mathcal{L}_i : V_i \mapsto \mathbb{R}^d$



where $L = \lceil log_2 |V| \rceil$ and $|V| = \sum_i^n |V_i|$ [Grauman 07].

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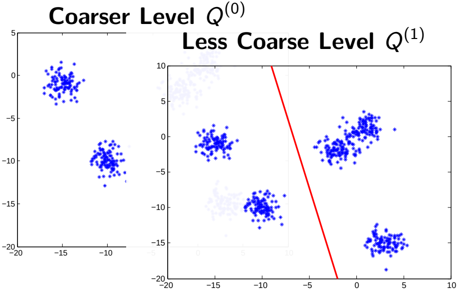

Coarser Level $Q^{(0)}$

Less Coarse Level $Q^{(1)}$

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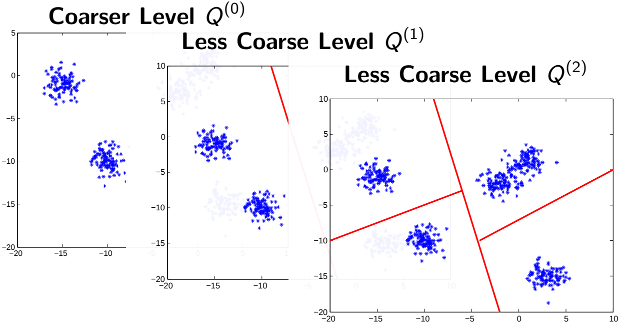

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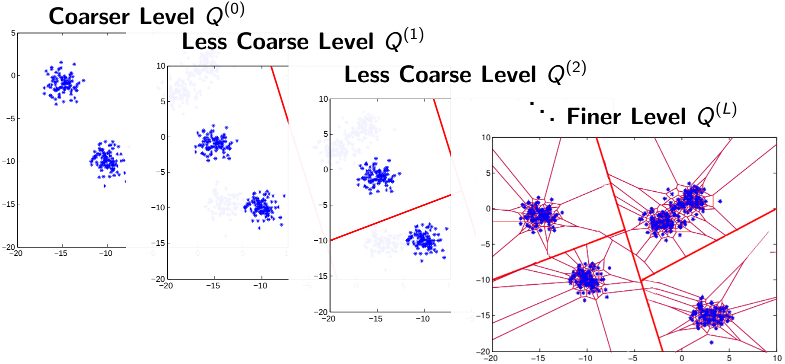


Coarser Level $Q^{(0)}$

Less Coarse Level $Q^{(1)}$

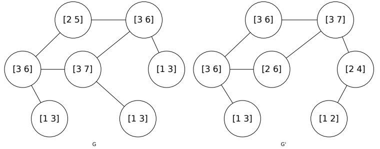
Less Coarse Level $Q^{(2)}$

$\ddots$ **Finer Level** $Q^{(L)}$

where $L = \lceil log_2 |V| \rceil$ and $|V| = \sum_i^n |V_i|$ [Grauman 07].

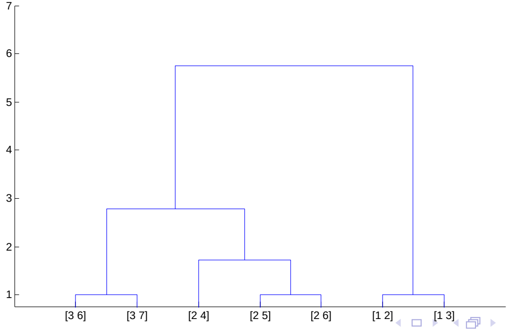
Data guided pyramid quantization scheme

Given labeled graphs G and G'



Notes

- Ward's minimum variance method over the image of V under $\mathcal{L}$.



Data guided pyramid quantization scheme

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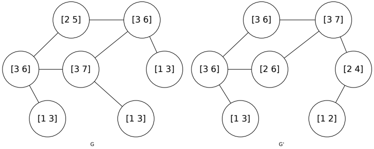
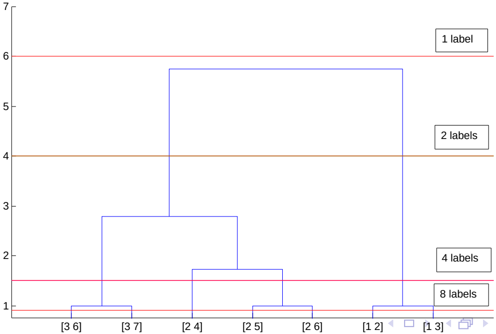


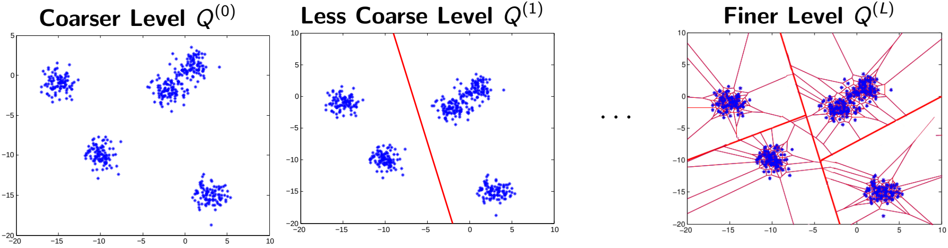
Notes

- Ward's minimum variance method over the image of V under $\mathcal{L}$.
- Selecting $L = \lceil log_2 D \rceil$, where $D \leq |V|$ the number of unique values in the image of V under $\mathcal{L}$
- Each level l has 2^l discrete labels.



Transform the initial graphs as a sequence of graphs

The pyramid quantization of label space



Coarser Level $Q^{(0)}$

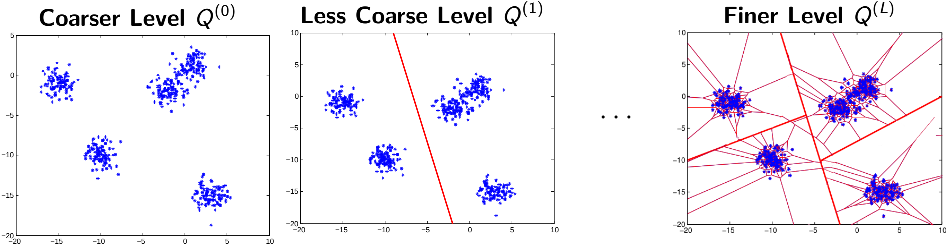
Less Coarse Level $Q^{(1)}$

. . .

Finer Level $Q^{(L)}$

Transform the initial graphs as a sequence of graphs

The pyramid quantization of label space



Coarser Level $Q^{(0)}$ **Less Coarse Level $Q^{(1)}$** . . . **Finer Level $Q^{(L)}$**

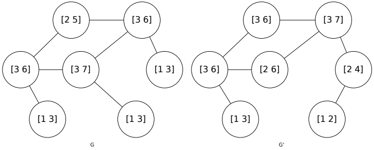
Sequence of discretely labeled graphs

$$G = (V, E, \mathcal{L}) \overset{Q^{(l)}\circ\mathcal{L}}{\underset{\forall l}{\approx}} \underset{\text{Increasing granularity}}{\underrightarrow{\left(G^{(0)}, \dots, G^{(L)}\right)}} = \underset{\text{Increasing granularity}}{\underrightarrow{\left((V, E, \mathcal{L}^{(0)}), \dots, (V, E, \mathcal{L}^{(L)})\right)}}$$

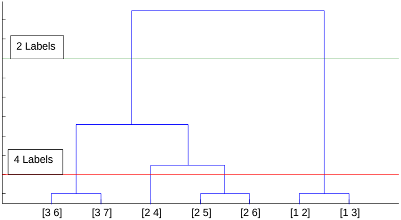
where $\mathcal{L}^{(l)} : V \rightarrow \Sigma_0^{(l)}$, $|\Sigma_0^{(l)}| = 2^l$ and $l \in \{0, \dots, L\}$.

A sequence of discretely labeled graphs

Given labeled graphs G and G'

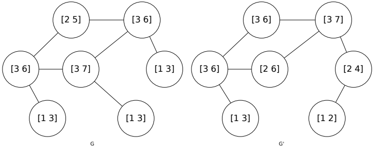


Data guided pyramid quantization.

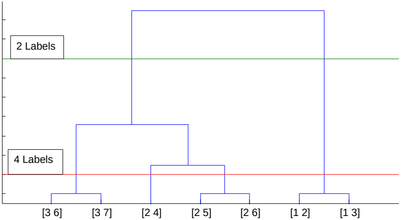


A sequence of discretely labeled graphs

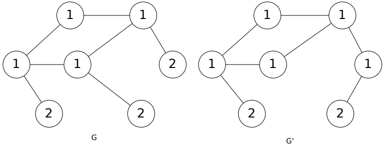
Given labeled graphs G and G'



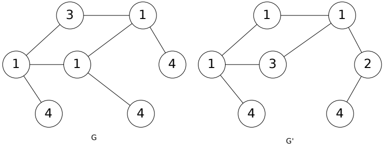
Data guided pyramid quantization.



Quantization level 1 with 2^1 number of labels.



Quantization level 2 with 2^2 number of labels



Creating and combining subtree features

Run Weisfeiler-Lehman on each quantization level

$$G = \left(G^{(0)}, \ldots, G^{(L)}\right) \xrightarrow[Lehman]{Weisfeler} \left(\phi^{(0)}_{(h)}(G^{(0)}), \ldots, \phi^{(L)}_{(h)}(G^{(L)})\right) = \widehat{\phi_{(h)}(G})$$

where $\phi^{(l)}_{(h)}(G^{(l)})$ are histograms of occurences of the subtree patterns up to depth h at the quantization level l in graph G

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Learning to combine the quantization levels

1. Learn the selection of the subtree features $\widehat{\phi_{(h)}(G)}$.
2. Combine the subtree features $\phi^{(l)}_{(h)}(G^{(l)})$ per level l into a kernel and then learn the combination of kernels.

Learn the subtree patterns selection

- Labeled training data $\{(\widehat{\phi_{(h)}(G_i)}, y_i)\}_{1 \leq i \leq n} \in (\mathbb{N} \times \mathbb{R})^n$ where
  - $\widehat{\phi_{(h)}(G_i)}$ is the concatination of histograms of the occurences of subtree patterns up to depth h of graph G_i across all quantization levels,
  - y_i is the ground truth label and

Learn the subtree patterns selection

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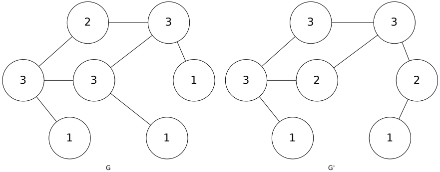
  - y_i is the ground truth label and
- Elastic Net [Zou 05]

$$\arg\min_{w \in \mathbb{R}^d} \underbrace{\lambda_1 \|w\|_1}_{\ell_1 \text{ norm}} + \underbrace{\lambda_2 \|w\|_2^2}_{\ell_2 \text{ norm}} + \underbrace{\frac{1}{n} \sum_{i=1}^{n} \left(\langle w, \widehat{\phi_{(h)}(G_i)} \rangle - y_i \right)^2}_{\text{Squared loss}}$$

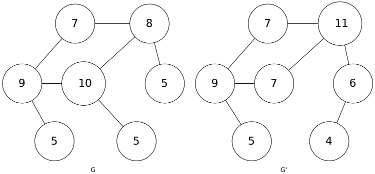
λ_1, λ_2 are scalar parameters controling the degree of regularization.

The intersection Weisfeiler-Lehman kernel

Subtree patterns of depth 0.



Subtree patterns of depth 1.



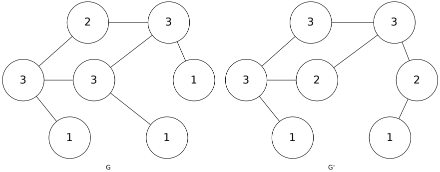
$$\text{Labels } \{\Sigma_0, \Sigma_1\} = \{\overbrace{1, \quad 2, \quad 3,}^{\text{Subtree patterns } h = 0} \quad \overbrace{4, \quad 5, \quad 6, \quad 7, \quad 8, \quad 9, \quad 10, \quad 11}^{\text{Subtree patterns } h = 1}\}$$

$$\phi^{(l)}_{(1)}(G^{(l)}) = (3, \quad 1, \quad 3, \quad 0, \quad 3, \quad 0, \quad 1, \quad 1, \quad 1, \quad 1, \quad 0)$$

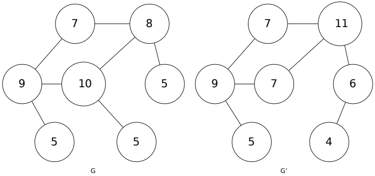
$$\phi^{(l)}_{(1)}(G'^{(l)}) = (2, \quad 2, \quad 3, \quad 1, \quad 1, \quad 1, \quad 2, \quad 0, \quad 1, \quad 0, \quad 1)$$

The intersection Weisfeiler-Lehman kernel

Subtree patterns of depth 0.



Subtree patterns of depth 1.



$$\begin{array}{rcl}
\text{Labels } \{\Sigma_0, \Sigma_1\} & = & \{\overbrace{1,\quad 2,\quad 3,}^{\text{Subtree patterns } h=0}\quad \overbrace{4,\quad 5,\quad 6,\quad 7,\quad 8,\quad 9,\quad 10,\quad 11}^{\text{Subtree patterns } h=1}\} \\
\phi^{(l)}_{(1)}(G^{(l)}) & = & (3,\quad 1,\quad 3,\quad 0,\quad 3,\quad 0,\quad 1,\quad 1,\quad 1,\quad 1,\quad 0) \\
\phi^{(l)}_{(1)}(G'^{(l)}) & = & (2,\quad 2,\quad 3,\quad 1,\quad 1,\quad 1,\quad 2,\quad 0,\quad 1,\quad 0,\quad 1) \\
\min\left(\phi^{(l)}_{(1)}(G^{(l)}), \phi^{(l)}_{(1)}(G'^{(l)})\right) & = & (2,\quad 1,\quad 3,\quad 0,\quad 1,\quad 0,\quad 1,\quad 0,\quad 1,\quad 0,\quad 0)
\end{array}$$

The intersection Weisfeile-Lehman kernel is defined :

$$k^{(h)}_{i-WLsubtree}(G^{(l)}, G'^{(l)}) = \sum_{j}^{|\Sigma_0 \cup \Sigma_1|} \min\left(\phi^{(l)}_{(1)}(G^{(l)}), \phi^{(l)}_{(1)}(G'^{(l)})\right)_j$$

Multiple Kernel Learning

Problem

For each pair of graphs $G^{(l)}, G'^{(l)}$ for all the pyramid levels:

$$\left(K_{(h)}^{(0)}(G^{(0)}, G'^{(0)}), \ldots, K_{(h)}^{(L)}(G^{(l)}, G'^{(L)})\right)$$

we would like to learn a linear combination of them:

$$K_{(h)}(G, G') = \sum_{l=0}^{L} d_l K_{(h)}^{(l)}(G^{(l)}, G'^{(l)}), \text{ with } d_l \geq 0, \sum_{l=0}^{L} d_l = 1.$$

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Solutions

- Multiple kernel learning
- Average weighted kernel

Table of Contents

fMRI Analysis

Key information

1. Inherent spatial structure brains
2. Voxel activation is a continuous value

fMRI Analysis

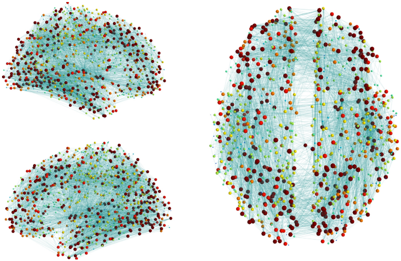
Key information

1. Inherent spatial structure brains
2. Voxel activation is a continuous value

⇓

Solution!

Represent fMRI as graphs with continuous labels.



Dataset

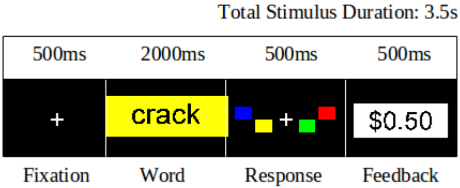
Cocaine Addiction Dataset

- 16 cocaine addicted vs 17 healthy subjects
- Drugstroop experiment with two varying conditions
  - the cue shown and
  - the monetary reward.

Input One contrast map per subject that is transformed into a graph.

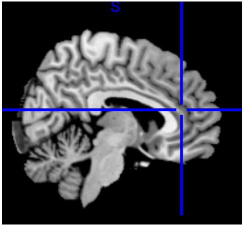
Objective The classification between cocaine abuser and control group.

Drugstroop Experiment



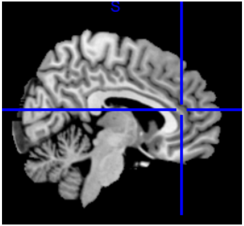
Graph Transformation

Contrast map



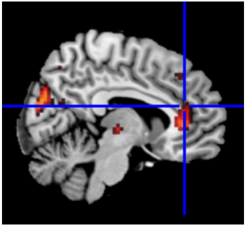
Graph Transformation

Contrast map



$$\xrightarrow{\text{Elastic Net}}$$

Selected voxels



Graph Transformation

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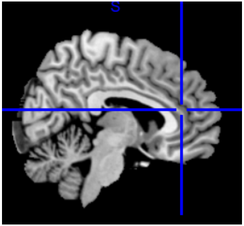

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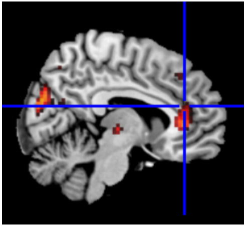
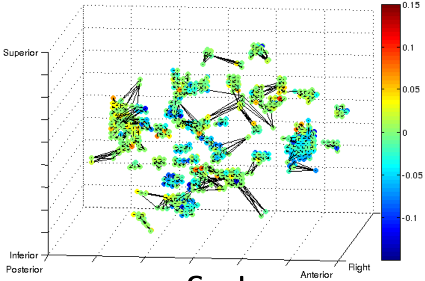
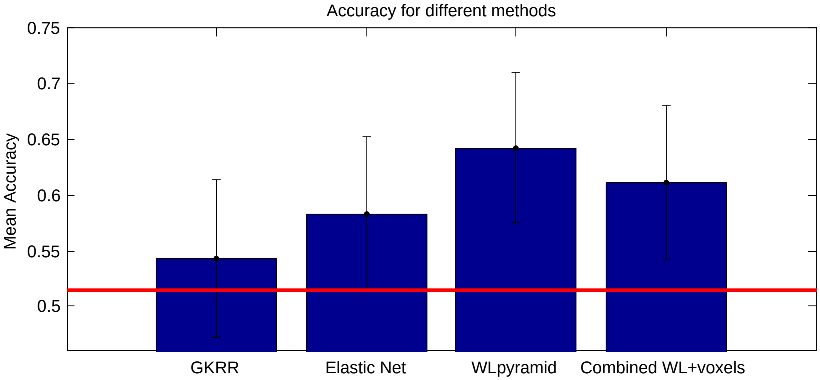


knn

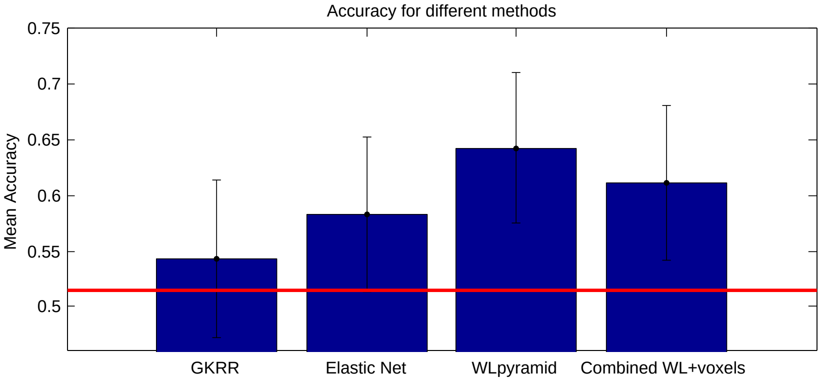


Graph

Performance



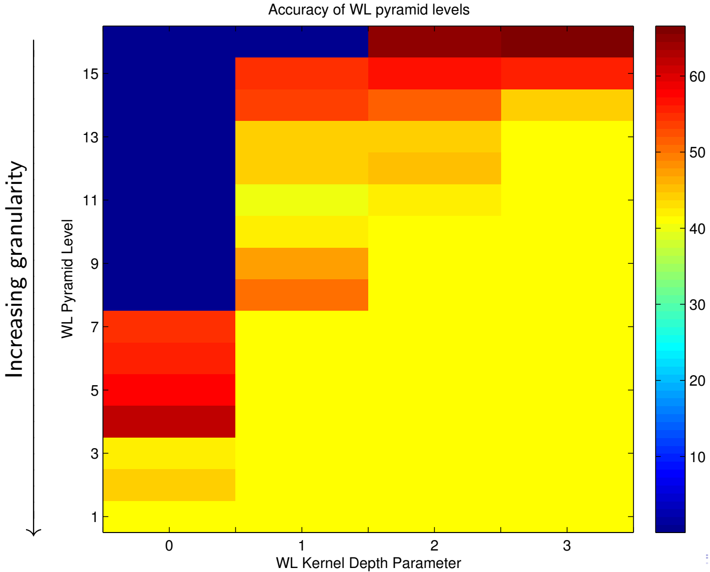
Performance



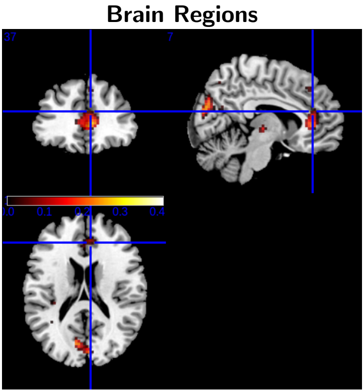
WLpyramid vs Elastic Net on raw voxels

Wilcoxon signed rank with $p = 0.02$ show statistical significance.

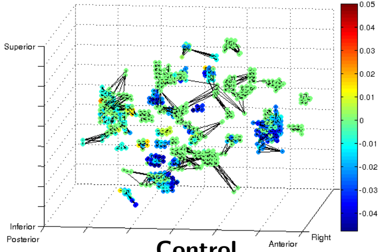
Performance per pyramid quantization level



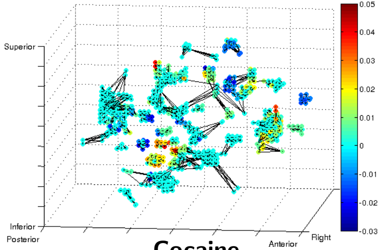
Visualization of learned function



Brain Regions



Control

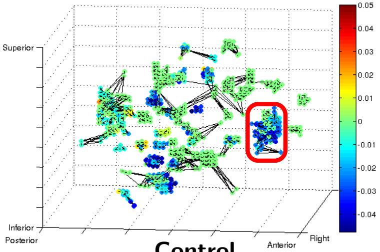


Cocaine

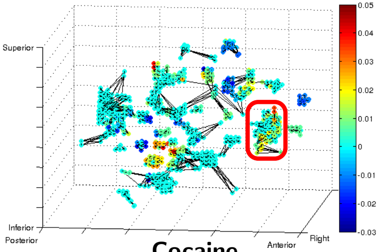
Visualization of learned function

Rostral Anterior Cingulate Cortex

- In cocaine addicted subjects deactivates during the drug Stroop experiment as compared to baseline.
- Its activity is normalized by oral methylphenidate where the dopamine transporters increase the extracellular dopamine, an increase which is associated with lower task-related impulsivity.



Control

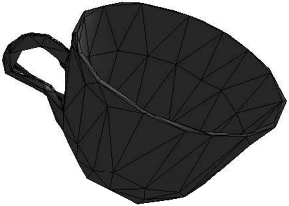


Cocaine

3D shape classification

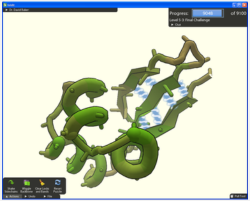
3D shape problems

- Storage
- Classification
- Retrieval

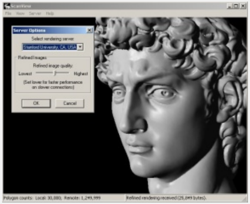


Areas of applications

3D Game



Chemoinformatics

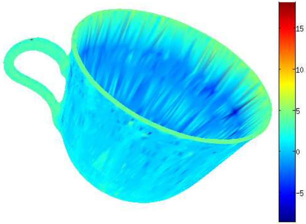


Cultural heritage

3D shape classification

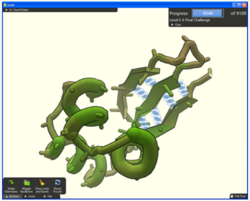
3D shape problems

- Storage
- Classification
- Retrieval



Areas of applications

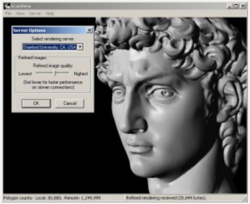
3D Game



Progress: 9048 of 9100

Level 5-3: Final Challenge

Chemoinformatics



Select rendering server: Stanford University, CA, USA

(Set lower for faster performance on slower connections)

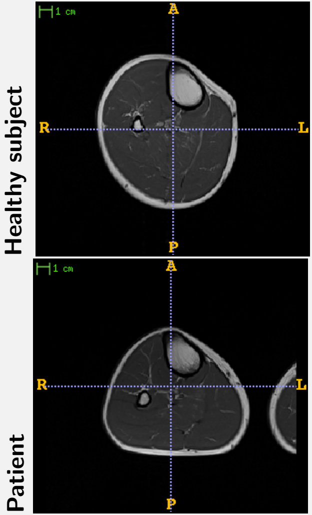
Polygon counts: Local: 30,000; Remote: 1,249,999

Refined rendering received (25,849 bytes).

Cultural heritage

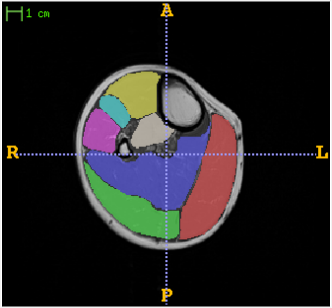
3D shape datasets

Muscle Dataset



3D shape datasets

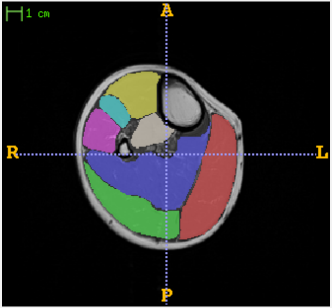
Muscle Dataset



- 27 patients vs 14 healthy subjects
- MRI images of the calf muscles
- Segmented into 7 muscles

3D shape datasets

Muscle Dataset



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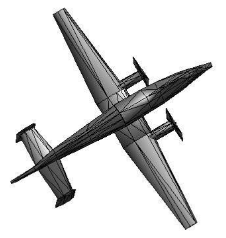
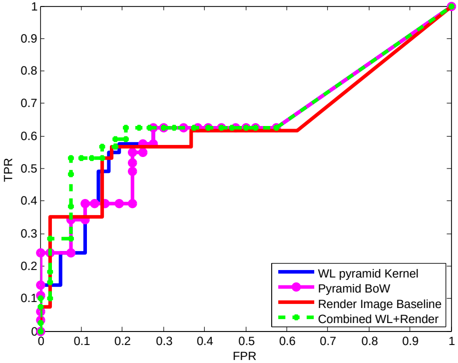
SHREC 2013 Dataset



- 20 classes of generic objects, such as bed, biplane, mug, etc.
- Each class contains 18 models.
- In total 360 3D objects.

Performance on the muscle dataset



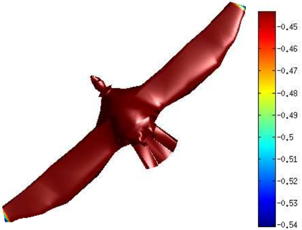
	WLpyramid Our Work	**pyramid BoW**	**Rendering**	**Combined**
Accuracy	78.00%	73.00%	75.50%	82.93%
AUC	0.6410	0.6361	0.6300	0.6648

Performance on SHREC 2013

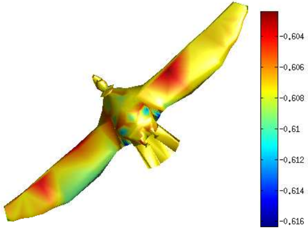
Class	WLpyramid Our Work	pyramid BoW	Rendering	Combined
Bird	0.85	0.83	0.85	**0.86**
Bicycle	0.84	0.87	0.90	0.90
Biped	0.89	0.88	0.99	0.99
Biplane	0.60	0.63	0.68	**0.69**
Bird	0.73	0.73	0.80	0.80
Bottle	0.76	0.76	0.79	**0.80**
Car	0.78	0.79	0.80	0.80
CellPhone	0.74	0.80	0.88	**0.89**
Chair	0.69	0.68	0.70	**0.72**
Cup	0.85	0.84	0.88	0.88
Desklamp	0.80	0.80	0.88	**0.89**
Fish	1.00	1.00	1.00	1.00
Floorlamp	0.80	0.77	0.89	0.89
Insect	0.64	0.60	0.62	**0.66**
Monoplane	0.84	0.82	0.88	**0.90**
Mug	0.82	0.82	0.85	**0.87**
Phone	0.83	0.74	0.72	**0.83**
Quadruped	0.89	0.86	0.97	**0.98**
Sofa	0.76	0.75	0.74	**0.75**
Wheelchair	0.81	0.79	0.88	**0.90**
Average	0.80	0.79	0.84	0.85

SHREC 2013 - Visualization of the learned weights

Subtree patterns of depth 0



Subtree patterns up to depth 2



Subtree patterns up to depth 1

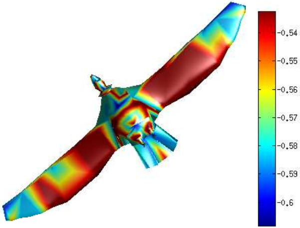


Table of Contents

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- Interpretation of 3D shape meshes as annotated graphs.

Future Work

Medical image analysis

- Evaluation of k-support norm regularization on fMRI analysis problem in larger scale.
- Evaluation of k-support regularized SVM on neuromuscular disease discrimination in larger scale.
- Exploration of different constructions of the graphs from fMRI.

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Graph kernels

- Comparison on partially matching subtree patterns.
- Comparison on partially labeled graphs.

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