Discrete Inference and Learning

Lecture 2
Primal-dual schema, dual decomposition

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Slides progressively constructed by
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Part I
Recap: MRFs and Convex Relaxations
Discrete MRF setting

• Given:
  – Objects from a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
  – The edges are undirected
  – A probability function

$$P(\mathcal{G}) = \prod_{v \in \mathcal{V}} P(v | \mathcal{N}_v)$$

• We can then state a wide range of problems on finding a set of assignments to maximize the probability $P$

$$\arg \max_{\mathcal{X}} P(\mathcal{G} | X) = \prod_{v_p \in \mathcal{V}} P(v = x_p | \mathcal{N}_v)$$

$$\arg \min_{\mathcal{X}} - \log P(\mathcal{G} | X) = \sum_p g_p(x_p) + \sum_{p, q : v_q \in \mathcal{N}_v_p} f_{p, q}(x_p, x_q)$$
Discrete MRF optimization

• Given:
  – Objects $\mathcal{V}$ from a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
  – If $X$ can be an assignment of discrete or continuous values

• Assign labels (to objects) that minimize MRF energy:

$$
\arg\min_{\chi} - \log P(\mathcal{G}|X) = \sum_{p} g_{p}(x_{p}) + \sum_{p,q: v_{q} \in \mathcal{N}_{v_{p}}} f_{p,q}(x_{p}, x_{q})
$$

- Unary potential
- Pairwise potential
Continuous MRF optimization

- Can be seen as a particular case of several machine learning scenarios with a specific prior
- Examples in computer vision and neuroimaging
  - Restoration
  - Functional brain activation
  - Optical flow
  - ...
- and beyond, connections with graph deep learning
- Comfortable way to express spatial priors
- Really powerful sound formulation
Continuous MRF optimization as common Regression (ML?) Problems

\[
\arg \min_{\mathcal{X}} - \log P(\mathcal{G} | \mathcal{X}) = \sum_p g_p(x_p) + \sum_{p,q: v_q \in \mathcal{N}_{v_p}} f_{p,q}(x_p, x_q)
\]

Regularized
\[
\arg \min_{\mathcal{X}} \quad d(Y, g(\mathcal{X})) + f(\mathcal{X})
\]

Ridge /Tik
\[
\arg \min_{\mathcal{X}} \quad \|Y - A\mathcal{X}\|^2_2 + \lambda \|\Gamma\mathcal{X}\|^2_2
\]

Lasso
\[
\arg \min_{\mathcal{X}} \quad \|Y - A\mathcal{X}\|^2_2 + \lambda \|\Gamma\mathcal{X}\|^1_1
\]

Elastic Net
\[
\arg \min_{\mathcal{X}} \quad \|Y - A\mathcal{X}\|^2_2 + \lambda_l \|\Gamma\mathcal{X}\|^1_1 + \lambda_r \|\Gamma\mathcal{X}\|^2_2
\]

These can be solved through quadratic programming [Hastie et al, Elements of Statistical Learning 2017]
Continuous MRF optimization as common Regression (ML?) Problems

$$\arg \min_{\mathbf{x}} - \log P(\mathcal{G}|\mathbf{X}) = \sum_{p} g_p(x_p) + \sum_{p,q: v_q \in \mathcal{N}_{v_p}} f_{p,q}(x_p, x_q)$$

$$\arg \min_{\mathbf{x}} \| \mathbf{Y} - A\mathbf{x} \|_2^2 + \lambda \| \Gamma \mathbf{x} \|_2^2$$

$$= \mathbf{Y}^T \mathbf{Y} + \mathbf{x}^T A^T A \mathbf{x} - 2 \mathbf{Y}^T A \mathbf{x} + \lambda \mathbf{x}^T \Gamma^T \Gamma \mathbf{x}$$

$$= \frac{1}{2} \mathbf{x}^T (A^T A + \lambda \Gamma^T \Gamma) \mathbf{x} - \mathbf{Y}^T A \mathbf{x}$$
Discrete MRF optimization

• Extensive research for more than 30 years

• MRF optimization ubiquitous in computer vision
  • segmentation
  • optical flow
  • image completion
  • stereo matching
  • image restoration
  • object detection/localization
  ...

• and beyond
  • medical imaging, computer graphics, digital communications, physics...

• Really powerful formulation
How to handle MRF optimization?

- Unfortunately, discrete MRF optimization is extremely hard (a.k.a. NP-hard)
  - E.g., highly non-convex energies

![MRF hardness diagram]

- Local optimum
- Global optimum
- Metric approximation
- Exact global optimum
- Linear
- Metric
- Arbitrary
How to handle MRF optimization?

We want:
Move right in the horizontal axis,
And remain low in the vertical axis
(i.e. still be able to provide approximately optimal solution)

We want to do it efficiently (fast)!
MRFs and Optimization

- Deterministic methods
  - Iterated conditional modes

- Non-deterministic methods
  - Mean-field and simulated annealing

- Graph-cut based techniques such as alpha-expansion
  - Min cut/max flow, etc.

- Message-passing techniques
  - Belief propagation networks, etc.
We would like to have a method which provides theoretical guarantees to obtain a good solution. Within a reasonably fast computational time.
Discrete optimization problems

\[
\min_{x} f(x) \quad \text{(optimize an objective function)}
\]

s.t. \( x \in C \quad \text{(subject to some constraints)} \)

this is the so called feasible set, containing all \( x \) satisfying the constraints

- Typically \( x \) lives on a very high dimensional space
How to handle MRF optimization?

- Unfortunately, discrete MRF optimization is extremely hard (a.k.a. NP-hard)
  - E.g., highly non-convex energies

- So what do we do?
  - Is there a principled way of dealing with this problem?

- Well, first of all, we don’t need to panic. Instead, we have to stay calm and RELAX!

- Actually, this idea of relaxing may not be such a bad idea after all...
The relaxation technique

- Very successful technique for dealing with difficult optimization problems

- It is based on the following simple idea:
  - try to approximate your original difficult problem with another one (the so called relaxed problem) which is easier to solve

- Practical assumptions:
  - Relaxed problem must always be easier to solve
  - Relaxed problem must be related to the original one
The relaxation technique

- True optimal solution
- Optimal solution to relaxed problem
- Feasible set
- Relaxed problem
How do we find easy problems?

- Convex optimization to the rescue

  "...in fact, the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity"

- Two conditions for an optimization problem to be convex:
  - convex objective function
  - convex feasible set
Why is convex optimization easy?

- Because we can simply let gravity do all the hard work for us

- More formally, we can let gradient descent do all the hard work for us
Why do we need the feasible set to be convex as well?

- Because, otherwise we may get stuck in a local optimum if we simply “follow gravity”
How do we get a convex relaxation?

- By dropping some constraints (so that the enlarged feasible set is convex)
- By modifying the objective function (so that the new function is convex)
- By combining both of the above
Linear programming (LP) relaxations

• Optimize linear function subject to linear constraints, i.e.:

\[
\begin{align*}
\min & \quad c^T x \\
\text{s.t.} & \quad Ax = b
\end{align*}
\]

• Very common form of a convex relaxation, because:
  • Typically leads to very efficient algorithms (important due to large scale nature of problems in computer vision)
  • Also often leads to combinatorial algorithms
  • Surprisingly good approximation for many problems
Geometric interpretation of LP

Max Z = 5X + 10Y
s.t.
X + 2Y <= 120
X + Y >= 60
X – 2Y >= 0
X, Y >= 0
MRFs and Linear Programming

• Tight connection between MRF optimization and Linear Programming (LP) recently emerged

• Active research topic with a lot of interesting work:
  
  – MRFs and LP-relaxations [Schlesinger] [Boros] [Wainwright et al. 05] [Kolmogorov 05] [Weiss et al. 07] [Werner 07] [Globerson et al. 07] [Kohli et al. 08]...
  
  – Tighter/alternative relaxations [Sontag et al. 07, 08] [Werner 08] [Kumar et al. 07, 08]
MRFs and Linear Programming

- E.g., state of the art MRF algorithms are now known to be directly related to LP:
  - Graph-cut based techniques such as \( a \)-expansion:
    generalized by primal-dual schema algorithms (Komodakis et al. 2005, 2007)
  - Message-passing techniques:
    further generalized by Dual-Decomposition (Komodakis 2007)

- The above statement is more or less true for almost all state-of-the-art MRF techniques
Part II
Primal-dual schema
The primal-dual schema

Highly successful technique for exact algorithms. Yielded exact algorithms for cornerstone combinatorial problems:
- matching
- network flow
- minimum spanning tree
- minimum branching
- shortest path
...

Soon realized that it’s also an extremely powerful tool for deriving approximation algorithms [Vazirani]:
- set cover
- steiner tree
- steiner network
- feedback vertex set
- scheduling
...

The primal-dual schema

- **Conjecture:**

  Any approximation algorithm can be derived using the primal-dual schema

  (has not been disproved yet)
The primal-dual schema

- Say we seek an optimal solution $x^*$ to the following integer program (this is our primal problem):
  \[
  \begin{align*}
  \text{min} \quad & c^T x \\
  \text{s.t.} \quad & Ax = b, \quad x \in \mathbb{N}
  \end{align*}
  \] (NP-hard problem)

- To find an approximate solution, we first relax the integrality constraints to get a primal & a dual linear program:
  \[
  \begin{align*}
  \text{primal LP:} \quad & \text{min} \quad c^T x \\
  \text{s.t.} \quad & Ax = b, \quad x \geq 0
  \end{align*}
  \]
  \[
  \begin{align*}
  \text{dual LP:} \quad & \text{max} \quad b^T y \\
  \text{s.t.} \quad & A^T y \leq c
  \end{align*}
  \]
Duality

\[
\begin{align*}
\text{min} & \quad 3x_1 + 2x_2 + 4x_3 \\
\text{subject to} & \quad 2x_1 + x_2 + x_3 \geq 2 \\
& \quad 2x_1 - x_2 + x_3 \geq 5 \\
\text{max} & \quad 2y_1 + 5y_2 \\
\text{subject to} & \quad 2y_1 + 2y_2 \leq 3 \\
& \quad y_1 - y_2 \leq 2 \\
& \quad y_2 \leq 4
\end{align*}
\]
Duality

\[
\begin{align*}
\text{min} & \quad 3x_1 + 2x_2 + 4x_3 \\
\text{subject to} & \\
2x_1 & + x_2 & + x_3 \quad \Rightarrow 2 \\
2x_1 & - x_2 & \quad \Rightarrow 5 \\
\text{max} & \quad 2y_1 + 5y_2 \\
\text{subject to} & \\
2y_1 & + 2y_2 \quad \Rightarrow 3 \\
y_1 & - y_2 \quad \Rightarrow 2 \\
y_2 \quad \Rightarrow 4
\end{align*}
\]
Duality

Theorem:
If the primal has an optimal solution, the dual has an optimal solution with the same cost.
The primal-dual schema

- **Goal:** find integral-primal solution $x$, feasible dual solution $y$ such that their primal-dual costs are “close enough”, e.g.,

\[
\frac{c^T x}{b^T y} \leq f^* \quad \text{and} \quad \frac{c^T x}{c^T x^*} \leq f^*
\]

Then $x$ is an $f^*$-approximation to optimal solution $x^*$
General form of the dual

\[
\begin{align*}
\text{min} & \quad c \ x \\
\text{subject to} & \quad a_i \ x = b_i \ (i \in E) \\
& \quad a_i \ x \geq b_i \ (i \in I) \\
& \quad x_j \geq 0 \ (j \in P) \\
& \quad x_j \in \mathcal{R} \ (j \in O)
\end{align*}
\]

Primal

\[
\begin{align*}
\text{max} & \quad y \ b \\
\text{subject to} & \quad y_i \in \mathcal{R} \ (i \in E) \\
& \quad y_i \geq 0 \ (i \in I) \\
& \quad yA_j \leq c_j \ (j \in P) \\
& \quad yA_j = c_j \ (j \in O)
\end{align*}
\]

Dual
Properties of Duality

- The dual of the dual is the primal

<table>
<thead>
<tr>
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Primal and Dual
Properties of Duality

- The dual of the dual is the primal

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Let $x$ and $\Pi$ be feasible solutions to the primal and dual respectively. We have that $cx \geq \Pi Ax \geq \Pi b$. 

Primal

Dual
## Properties of Duality

- The dual of the dual is primal

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Primal/Dual Relationships

\[
\begin{align*}
\text{min} & \quad x_1 \\
\text{subject to} & \quad x_1 + x_2 \geq 1 \\
& \quad -x_1 - x_2 \geq 1
\end{align*}
\]

infeasible primal

\[
\begin{align*}
\text{max} & \quad y_1 + y_2 \\
\text{subject to} & \quad y_1 - y_2 = 1 \\
& \quad y_1 - y_2 = 0 \\
& \quad y_i \geq 0
\end{align*}
\]

infeasible dual
Primal/Dual Relationships

min
subject to
\[ x_1 \]
\[ x_1 + x_2 \geq 1 \]
\[ -x_1 - x_2 \geq 1 \]
\[ x_j \geq 0 \]
infeasible primal

max
subject to
\[ y_1 + y_2 \]
\[ y_1 - y_2 \leq 1 \]
\[ y_1 - y_2 \leq 0 \]
\[ y_i \geq 0 \]
unbounded dual
Certificate of Optimality

- NP-complete problems
  - Certificate of feasibility

- Can you provide
  - A certificate of optimality?

- Consider now a linear program
  - Can you convince me that you have found an optimal solution?
Certificate of Optimality

primal

\[
\begin{align*}
\text{min} & \quad c \ x \\
\text{subject to} & \quad Ax \geq b \\
& \quad x_j \geq 0
\end{align*}
\]

dual

\[
\begin{align*}
\text{max} & \quad y \ b \\
\text{subject to} & \quad yA \leq c \\
& \quad y \geq 0
\end{align*}
\]

- Give me a \( x^* \) that satisfies \( A x^* \geq b \)
- Give me a \( y^* \) that satisfies \( y^* A \leq c \)
- Show me that \( c x^* = y^* b \).
Bounding

\[
\begin{align*}
\text{max} & \quad 4x_1 + x_2 + 5x_3 + 3x_4 \\
\text{subject to} & \quad x_1 - x_2 - x_3 + 3x_4 \leq 1 \\
& \quad 5x_1 + x_2 + 3x_3 + 8x_4 \leq 55 \\
& \quad -x_1 + 2x_2 + 3x_3 - 5x_4 \leq 3
\end{align*}
\]

\[\text{can we find an upper bound?}\]

\[
10x_1 + 2x_2 + 6x_3 + 16x_4 \leq 110
\]
Bounding

\[ \begin{align*}
\text{max} & \quad 4x_1 + x_2 + 5x_3 + 3x_4 \\
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**can we find an upper bound?**

\[
\begin{align*}
10x_1 + 2x_2 + 6x_3 + 16x_4 & \leq 110 \\
4x_1 + 3x_2 + 6x_3 + 3x_4 & \leq 58
\end{align*}
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Bounding

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• positive combinations of the constraints
Bounding

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\end{align*}
\]

\[\begin{bmatrix}
y_1 \\
y_2 \\
y_3
\end{bmatrix}\]

- positive combinations of the constraints
Bounding

\[ \text{max} \quad 4x_1 + x_2 + 5x_3 + 3x_4 \]
subject to
\[ x_1 - x_2 - x_3 + 3x_4 \leq 1 \]
\[ 5x_1 + x_2 + 3x_3 + 8x_4 \leq 55 \]
\[ -x_1 + 2x_2 + 3x_3 - 5x_4 \leq 3 \]

\[ \text{positive combinations of the constraints} \]
\[ y_1 \left( x_1 - x_2 - x_3 + 3x_4 \right) + \]
\[ y_2 \left( 5x_1 + x_2 + 3x_3 + 8x_4 \right) + \]
\[ y_3 \left( -x_1 + 2x_2 + 3x_3 - 5x_4 \right) \leq \]
\[ y_1 + 55y_2 + 3y_3 \]
Bounding

\[
\begin{align*}
\text{max} & \quad 4x_1 + x_2 + 5x_3 + 3x_4 \\
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\]

- positive combinations of the constraints

\[
\begin{align*}
y_1 & \quad (x_1 - x_2 - x_3 + 3x_4) + \\
y_2 & \quad (5x_1 + x_2 + 3x_3 + 8x_4) + \\
y_3 & \quad (-x_1 + 2x_2 + 3x_3 - 5x_4) \leq \\
\end{align*}
\]

minimize \( y_1 + 55y_2 + 3y_3 \)
Complementarity slackness

Let $x^*$ and $y^*$ be the optimal solutions to the primal and dual. The following conditions are necessary and sufficient for the optimality of $x^*$ and $y^*$:

\[
\sum_{j=1}^{n} a_{ij} x_j^* = b_i \lor y_i^* = 0 \quad (1 \leq i \leq m)
\]

\[
\sum_{i=1}^{n} a_{ij} y_i^* = c_j \lor x_j^* = 0 \quad (1 \leq j \leq n)
\]
Economic Interpretation

Maximizing profit:

$$\max \sum_{j=1}^{n} c_j x_j$$

subject to

$$\sum_{j=1}^{n} a_{ij} x_j \leq b_i + t_i \quad (1 \leq i \leq m)$$

Capacity constraints on your production:

- for some small $t_i$, this linear program has an optimal solution

$$z^* + \sum_{i=1}^{m} y_i^* t_i$$

optimal primal objective  dual solution
Primal-Dual

- Why using the dual?
  - I have an optimal solution and I want to add a new constraint
  - The dual is still feasible (I am adding a new variable); the primal is not
  - Optimize the dual and the primal becomes feasible at optimality
The primal-dual schema

- The primal-dual schema works iteratively

  sequence of dual costs

  sequence of primal costs

  \[
  \begin{align*}
  c^T x^k & \leq f^* \\
  b^T y^k & \leq f^*
  \end{align*}
  \]

- Global effects, through local improvements!

- Instead of working directly with costs (usually not easy), use relaxed complementary slackness conditions (easier)

- Different relaxations of complementary slackness
  Different approximation algorithms!!!
The primal-dual schema for MRFs

\[
\min \left[ \sum_{p \in G} \sum_{a \in L} V_p(a) x_{p,a} + \sum_{pq \in E} \sum_{a,b \in L} V_{pq}(a, b) x_{pq,ab} \right]
\]

s.t. \( \sum_{a \in L} x_{p,a} = 1 \) (only one label assigned per vertex)

\[
\begin{align*}
\sum_{a \in L} x_{pq,ab} &= x_{q,b} \\
\sum_{b \in L} x_{pq,ab} &= x_{p,a}
\end{align*}
\]

\( x_{p,a} \geq 0, \ x_{pq,ab} \geq 0 \)

Binary variables

\[
\begin{align*}
x_{p,a} &= 1 &\iff& \text{label } a \text{ is assigned to node } p \\
x_{pq,ab} &= 1 &\iff& \text{labels } a, b \text{ are assigned to nodes } p, q
\end{align*}
\]
Complementary slackness

primal LP: \[ \min c^T x \]
\[ \text{s.t. } Ax = b, x \geq 0 \]
dual LP: \[ \max b^T y \]
\[ \text{s.t. } A^T y \leq c \]

Complementary slackness conditions:

\[ \forall 1 \leq j \leq n : \quad x_j > 0 \Rightarrow \sum_{i=1}^{m} a_{ij} y_i = c_j \]

Theorem. If \( x \) and \( y \) are primal and dual feasible and satisfy the complementary slackness condition then they are both optimal.
Relaxed complementary slackness

primal LP: \[ \min c^T x \]
\[ \text{s.t. } A x = b, x \geq 0 \]
dual LP: \[ \max b^T y \]
\[ \text{s.t. } A^T y \leq c \]

Exact CS:
\[ \forall 1 \leq j \leq n : \quad x_j > 0 \Rightarrow \sum_{i=1}^{m} a_{ij} y_i = c_j \]

Relaxed CS:
\[ \forall 1 \leq j \leq n : \quad x_j > 0 \Rightarrow \sum_{i=1}^{m} a_{ij} y_i \geq c_j / f_j \]

implies 'e

\[ f_j = 1 \forall j \]

Theorem. If \( x, y \) primal/dual feasible and satisfy the relaxed CS condition then \( x \) is an \( f \)-approximation of the optimal integral solution, where \( f = \max_j f_j \).
Complementary slackness and the primal-dual schema

Theorem (previous slide). If $x, y$ primal/dual feasible and satisfy the relaxed CS condition then $x$ is an $f$-approximation of the optimal integral solution, where $f = \max_j f_j$.

Goal of the primal dual schema: find a pair $(x, y)$ that satisfies:
- Primal feasibility
- Dual feasibility
- (Relaxed) complementary slackness conditions.
Regarding the PD schema for MRFs, it turns out that:

- Each update of primal and dual variables solving max-flow in appropriately constructed graph

Resulting flows tell us how to update both:
- the dual variables, as well as
- the primal variables

Max-flow graph defined from current primal-dual pair \( (x^k,y^k) \)
- \( (x^k,y^k) \) defines connectivity of max-flow graph
- \( (x^k,y^k) \) defines capacities of max-flow graph

Max-flow graph is thus continuously updated
FastPD: primal-dual schema for MRFs

- Very general framework. Different PD-algorithms by RELAXING complementary slackness conditions differently.

- E.g., simply by using a particular relaxation of complementary slackness conditions (and assuming $V_{pq}(\cdot,\cdot)$ is a metric)
  THEN resulting algorithm shown equivalent to a-expansion!
  [Boykov, Veksler, Zabih]

- PD-algorithms for non-metric potentials $V_{pq}(\cdot,\cdot)$ as well

- Theorem: All derived PD-algorithms shown to satisfy certain relaxed complementary slackness conditions

- **Worst-case** optimality properties are thus guaranteed
Per-instance optimality guarantees

- Primal-dual algorithms can always tell you (for free) how well they performed for a particular instance.

\[ r_2 = \frac{c^T x^2}{b^T y^2} \]

- Per-instance approx. factor
- Per-instance upper bound
- Per-instance lower bound (per-instance certificate)
- Unknown optimum
Computational efficiency (static MRFs)

- MRF algorithm only in the primal domain (e.g., a-expansion)
  - Fixed dual cost
  - Many augmenting paths per max-flow
  - Primal-dual gap = upper-bound on #augmenting paths per max-flow

- MRF algorithm in the primal-dual domain (Fast-PD)
  - Few augmenting paths per max-flow

Theorem: primal-dual gap = upper-bound on #augmenting paths (i.e., primal-dual gap indicative of time per max-flow)
Computational efficiency (static MRFs)

- Incremental construction of max-flow graphs (recall that max-flow graph changes per iteration)

- Possible because we keep both primal and dual information

- Principled way for doing this construction via the primal-dual framework
Computational efficiency (static MRFs)

- *penguin* almost constant
- *Tsukuba* dramatic decrease
- *SRI-tree*
Computational efficiency (dynamic MRFs)

- Fast-PD can speed up dynamic MRFs [Kohli,Torr] as well (demonstrates the power and generality of this framework)

  ![Diagram of Fast-PD algorithm]

- Principled (and simple) way to update dual variables when switching between different MRFs
Drop: Deformable Registration using Discrete Optimization [Glocker et al. 07, 08]

- Easy to use GUI
- Main focus on medical imaging
- 2D-2D registration
- 3D-3D registration
- Publicly available: http://campar.in.tum.de/Main/Drop
primal-dual framework

- New theorems
- New insights into existing techniques
- New view on MRFs

Handles wide class of MRFs

Approximately optimal solutions

Significant speed-up for dynamic MRFs

Significant speed-up for static MRFs

Theoretical guarantees AND tight certificates per instance
Take home message:

LP and its duality theory provides:

- Powerful framework for systematically tackling the MRF optimization problem
- Unifying view for the state-of-the-art MRF optimization techniques