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Newton update in L_2-norm random tree approximation

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Preliminaries

- $\mathcal{X}$ is an arbitrary input space, $\mathbf{x} \in \boldsymbol{\mathcal{X}}$.
- $\mathcal{Y}$ is an output space of a set of ℓ-dimensional *multilabels*

$$\mathbf{y} = (y_1, \cdots, y_\ell) \in \boldsymbol{\mathcal{Y}}.$$

- y_i is a *microlabel* and $y_i \in \{1, \cdots, r_i\}, r_i \in \mathbb{Z}$.
- For example, multilabel binary classification $y_i \in \{-1, +1\}$.
- Training examples are sampled from $(\mathbf{x}, \mathbf{y}) \in \boldsymbol{\mathcal{X}} \times \boldsymbol{\mathcal{Y}}$.
- Each example $(\mathbf{x}, \mathbf{y})$ is mapped into a joint feature space $\boldsymbol{\phi}(\mathbf{x}, \mathbf{y})$.
- $\mathbf{w}$ is the weight vector in the joint feature space.
- Define a linear score function $F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle$.
- The prediction $\mathbf{y}_\mathbf{w}(\mathbf{x})$ of an input $\mathbf{x}$ is the multilabel $\mathbf{y}$ that maximizes the score function

$$\mathbf{y}_\mathbf{w}(\mathbf{x}) = \operatorname*{\mathbf{argmax}}_{\mathbf{y} \in \boldsymbol{\mathcal{Y}}} \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle. \tag{1}$$

- (1) is called *inference* problem which is $\mathcal{NP}$-hard for most output feature maps.

Markov network

- We assume that the joint feature map $\boldsymbol{\phi}$ is a potential function on a Markov network $G = (E, V)$.
- G is a complete graph with $|V| = \ell$ nodes and $|E| = \frac{\ell(\ell-1)}{2}$ undirected edges.
- G models all pairwise correlations.
- $\boldsymbol{\varphi}(\mathbf{x})$ is the input feature map, e.g., bag-of-words feature of an example $\mathbf{x}$.
- $\boldsymbol{\psi}(\mathbf{y})$ is the output feature map which is a collection of edges and labels

$$\boldsymbol{\varphi}(\mathbf{y}) = (u_e)_{e\in E}, u_e \in \{-1, +1\}^2.$$

- The joint feature is the Kronecker product of $\boldsymbol{\varphi}(\mathbf{x})$ and $\boldsymbol{\psi}(\mathbf{y})$

$$\boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) = (\boldsymbol{\phi}_e(\mathbf{x}, \mathbf{y}))_{e\in E} = (\boldsymbol{\varphi}(\mathbf{x}) \otimes \boldsymbol{\psi}_e(\mathbf{y}_e))_{e\in E}.$$

- The score function can be factorized by the complete graph G

$$F(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \langle \mathbf{w}, \boldsymbol{\phi}(\mathbf{x}, \mathbf{y}) \rangle = \sum_{e\in E} \langle \mathbf{w}_e, \boldsymbol{\phi}_e(\mathbf{x}, \mathbf{y}_e) \rangle.$$

Inference in terms of all spanning trees

- Solving the following inference problem on a complete graph is $\mathcal{NP}$-hard

$$\mathbf{y}_{\mathbf{w}}(\mathbf{x}) = \underset{\mathbf{y}\in\mathcal{Y}}{\mathbf{argmax}}\, F(\mathbf{w},\mathbf{x},\mathbf{y}) = \underset{\mathbf{y}\in\mathcal{Y}}{\mathbf{argmax}} \sum_{e\in E} \langle \mathbf{w}_e, \boldsymbol{\phi}_e(\mathbf{x},\mathbf{y}_e)\rangle.$$

- For a complete graph, there are $\ell^{\ell-2}$ unique spanning trees.
- We can write $F(\mathbf{w},\mathbf{x},\mathbf{y})$ as a conic combination of all spanning trees

$$F(\mathbf{w},\mathbf{x},\mathbf{y}) = \underset{T\in U(G)}{\mathbf{E}} a_T \langle \mathbf{w}_T, \boldsymbol{\phi}_T(\mathbf{x},\mathbf{y})\rangle$$
$$\underset{T\in U(G)}{\mathbf{E}} a_T^2 = 1,\ \underset{T\in U(G)}{\mathbf{E}} a_T < 1.$$

- $U(G)$ is the uniform distribution over $\ell^{\ell-2}$ spanning trees.
- The number of spanning trees is exponentially dependent on the number of nodes ℓ.

A sample of n spanning trees

- Instead of using all spanning trees, we can just use n spanning trees

$$F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \frac{1}{n} \sum_{i=1}^{n} a_{T_i} \langle \mathbf{w}_{T_i}, \boldsymbol{\phi}_{T_i}(\mathbf{x}, \mathbf{y}) \rangle$$

$$\frac{1}{n} \sum_{i=1}^{n} a_{T_i}^2 = 1, \frac{1}{n} \sum_{i=1}^{n} a_{T_i} < 1.$$

- When

$$n \geq \frac{\ell^2}{\epsilon^2} \left(\frac{1}{16} + \frac{1}{2} \ln \frac{8\sqrt{n}}{\delta} \right),$$

  we have $|F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y}) - F(\mathbf{w}, \mathbf{x}, \mathbf{y})| \leq \epsilon$, with high probability.

- A sample of $n \in \Theta(\ell^2/\delta^2)$ random spanning tree is sufficient to estimate the score function.
- Margin achieved by $F(\mathbf{w}, \mathbf{x}, \mathbf{y})$ is also preserved by the sample of n random spanning trees $F_{\mathcal{T}}(\mathbf{w}, \mathbf{x}, \mathbf{y})$.

Optimization problem

- The primal optimization problem is defined as

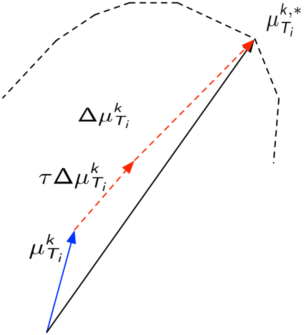
$$\begin{aligned}
\min_{\mathbf{w}_{T_i},\xi_i} \quad & \frac{1}{2}\sum_{i=1}^{n} ||\mathbf{w}_{T_i}||^2 + C\sum_{k=1}^{m}\xi_k \\
\textbf{s.t.} \quad & \sum_{i=1}^{n} \langle \mathbf{w}_{T_i}, \Delta\boldsymbol{\phi}_{T_t}(\mathbf{x}_k,\mathbf{y}_k)\rangle \geq \ell_{T_i,k} - \xi_k, \\
& \xi_k \geq 0\,, \forall\ k \in \{1,\dots,m\}.
\end{aligned}$$

- The marginalized dual problem is defined as

$$\begin{aligned}
\max_{\mu\in\mathcal{M}} \quad & \sum_{i=1}^{n}\left(\mu_{T_i}\boldsymbol{\ell}_{T_i} - \frac{1}{2}\mu_{T_i}K_{T_i}^{\Delta\boldsymbol{\phi}}\mu_{T_i}\right) \\
\textbf{s.t.} \quad & \sum_{u_e}\mu_{T_i,e}(u_e) \leq C.
\end{aligned}$$

- How to optimize a collection of n spanning trees jointly?

Optimization on a single random spanning tree T_i



Optimization on a single random spanning tree T_i

- The optimization problem can be solved efficiently on a single tree T_i.
- The algorithm iterates over all training examples until convergence.
- We drop the index momentarily $\mu \leftarrow \mu(j)$, $g \leftarrow g(j)$, $\ell \leftarrow \ell(j)$.
- For the kth iteration:
  1. Obtain the current solution of the jth example $\mu^k_{T_i}$.
  2. Compute the current gradient on $\mu^k_{T_i}$, $g^k_{T_i} = \ell_{T_i} - K^{\Delta\phi}_{T_i}\mu^k_{T_i}$.
  3. Compute a feasible solution $\mu^{k,*}_{T_i}$ as an update direction (efficiently)
  $$\mu^{k,*}_{T_i} = \underset{\mu \in \mathcal{M}}{\mathbf{argmax}}\, \mu^\intercal g^k_{T_i}. \quad (2)$$
  4. Compute an update direction from the current solution $\mu^k_{T_i}$ towards the feasible solution $\mu^{k,*}_{T_i}$
  $$\Delta\mu^k_{T_i} = \mu^{k,*}_{T_i} - \mu^k_{T_i}.$$
  5. Compute a stationary point (τ) and perform the update
  $$\mu^{k+1}_{T_i} = \mu^k_{T_i} + \tau\Delta\mu^k_{T_i}.$$

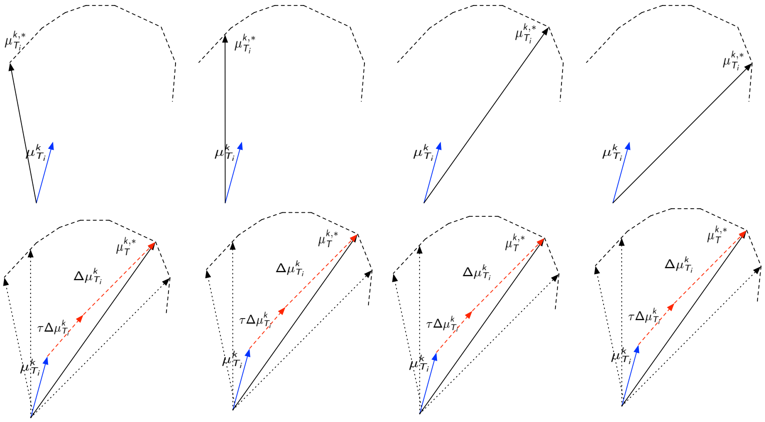
Exact line search for a single tree

- Line search gives the optimal feasible solution as a stationary point (τ)

$$\begin{aligned} \max_{\tau} \quad & f(\mu^k_{T_i} + \tau \Delta \mu^k_{T_i}) \\ \textbf{s.t.} \quad & 0 \leq \tau \leq 1. \end{aligned} \tag{3}$$

- $\tau = 0$ corresponds to no update.
- Feasible maximum update is achieved at $\tau = 1$.
- The cost of computing (3) is significantly smaller than the cost of computing (2).

Optimization on a collection of n spanning trees



Optimization on a collection of n spanning trees

- The algorithm iterates over all training examples until convergence.
- We drop the index momentarily $\mu \leftarrow \mu(j)$, $g \leftarrow g(j)$, $\ell \leftarrow \ell(j)$.
- For the kth iteration:
  1. Obtain the current solutions over all spanning trees $(\mu_{T_i}^k)_{i=1}^n$.
  2. Compute the gradients over all trees $(g_{T_i}^k)_{i=1}^n$.
  3. Compute a feasible solution for each individual spanning tree
  $$\mu_{T_i}^{k,*} = \operatorname*{\mathbf{argmax}}_{\mu \in \mathcal{M}} \mu^\intercal g_{T_i}^k, \ \forall i.$$
  4. Compute the best feasible solution over the collection
  $$\mu_T^{k,*} = \operatorname*{\mathbf{argmax}}_{\mu \in (\mu_{T_i}^{k,*})_{i=1}^n} \sum_{i=1}^n \mu^\intercal g_{T_i}^k$$
  5. Compute the update direction
  $$\Delta\mu_{T_i}^k = \mu_{T_i}^k - \mu_T^{k,*}, \ \forall i.$$
  6. Perform the update to the optimal feasible solution
  $$\mu_{T_i}^{k+1} = \mu_{T_i}^k + \tau\Delta\mu_{T_i}^k, \ \forall i.$$

Exact line search for the collection of trees

- The step size along the update direction τ is given by the exact line search

$$\begin{aligned} \max_{\tau} \quad & \sum_{i=1}^{n} f(\mu^k_{T_i} + \tau\Delta\mu^k_{T_i}) \\ \textbf{s.t.} \quad & 0 \leq \tau \leq 1. \end{aligned}$$

- Problems with the *best update*
  1. The best feasible solution on a single tree might not be the best feasible solution on a collection of trees

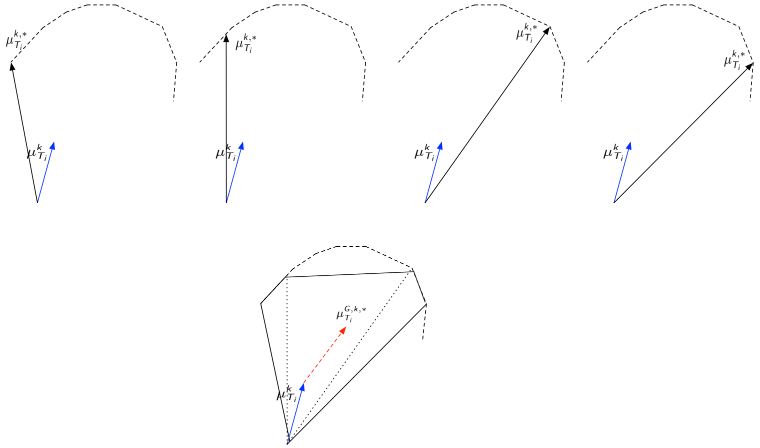
$$\mu^{k,*}_{T} \notin (\mu^{k,*}_{T_i})_{i=1}^{n}.$$

  2. κ-best inference algorithm

$$(\mu^{k,*_h}_{T_i})_{h=1}^{\kappa} = \operatorname*{\mathbf{argmax}}_{\mu \in \mathcal{M}} \mu^{\intercal} g^k_{T_i}, \ \forall i$$

$$\mu^{k,*}_{T} \in (\mu^{k,*_h}_{T_i})_{i=\{1,\cdots,n\},h\in\{1,\cdots,\kappa\}}.$$

Update with multiple directions



Update with multiple directions

- The algorithm iterates over all training examples until convergence.
- We drop the index momentarily $\mu \leftarrow \mu(j)$, $g \leftarrow g(j)$, $\ell \leftarrow \ell(j)$.
- For the kth iteration:
  1. Obtain the current solutions over all spanning trees $(\mu_{T_i}^{k})_{i=1}^{n}$.
  2. Compute the gradients over all trees $(g_{T_i}^{k})_{i=1}^{n}$.
  3. Compute a feasible solution for each individual spanning tree
  $$\mu_{T_i}^{k,*} = \operatorname*{\mathbf{argmax}}_{\mu \in \mathcal{M}} \mu^{\mathsf{T}} g_{T_i}^{k}, \ \forall i.$$
  4. Project each local feasible solution to a global feasible solution
  $$\mu_{T_i}^{G,k,*} \leftarrow \mu_{T_i}^{k,*}, \ \forall i.$$
  5. Define a convex combination of update directions
  $$\Delta\mu^{G,k} = \sum_{i=1}^{n} \tau_i \Delta\mu_{T_i}^{G,k,*} = \sum_{i=1}^{n} \tau_i \left(\mu^{G,k} - \mu_{T_i}^{G,k,*}\right).$$
  6. Perform the update $\mu^{G,k+1} = \mu^{G,k} + \Delta\mu^{G,k+1}$.
  7. Project the global solution on spanning trees $(\mu_{T_i}^{k+1})_{i=1}^{n} \leftarrow \mu^{G,k+1}$.

Newton method to compute τ

- We want to find τ that maximize the objective function given the update

$$\max_{\tau} \quad f(\mu^{G,k} + \Delta\mu^{G,k+1})$$
$$\textbf{s.t.} \quad 0 \leq \tau_i \leq 1, \sum_{i=1}^{n} \tau_i \leq 1, \forall i.$$

- The objective is quadratic with respect to $\boldsymbol{\tau}$.
- We use Newton method to find $\boldsymbol{\tau}$ that maximize the objective.
- $\boldsymbol{\tau}$ is projected into the feasible region.

Compute duality gap

- We use duality gap to measure the progress of the optimization.
- Primal and dual objective function

$$f(\mathbf{w}) = \frac{1}{2}||\mathbf{w}||^2 + C\sum_{i=1}^{m}(\ell_i - \langle \mathbf{w}, \Delta\boldsymbol{\phi}(\mathbf{x}_i, \mathbf{y}_i)\rangle)$$

$$g(\boldsymbol{\alpha}) = \sum_{i=1}^{m}\alpha_i\ell_i - \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha_i K^{\Delta\boldsymbol{\phi}}(\mathbf{x}_i, \mathbf{y}_i; \mathbf{x}_j, \mathbf{y}_j)\alpha_j$$

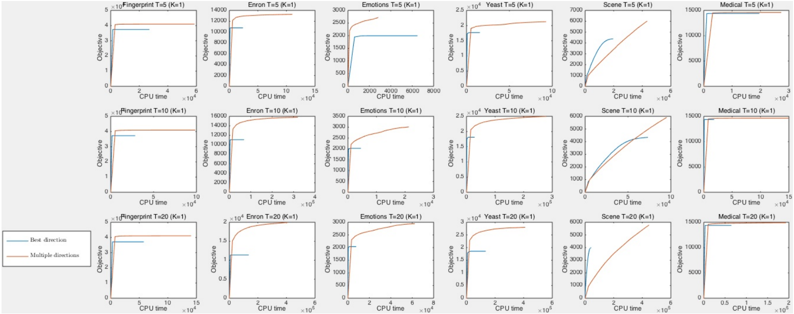
- $\max\limits_{\boldsymbol{\alpha}} g(\boldsymbol{\alpha}) \leq \min\limits_{\mathbf{w}} f(\mathbf{w})$, minimum gap when optimal.
- Duality gap at $\boldsymbol{\alpha}^k$

$$\begin{aligned} f(\mathbf{w}^k) - g(\boldsymbol{\alpha}^k) &= C\left(\boldsymbol{\ell} - K^{\Delta\boldsymbol{\phi}}\boldsymbol{\alpha}^k\right) - \boldsymbol{\alpha}^k\left(\boldsymbol{\ell} - K^{\Delta\boldsymbol{\phi}}\boldsymbol{\alpha}^k\right) \\ &= C^{\mathsf{T}}\nabla g(\boldsymbol{\alpha}^k) - \boldsymbol{\alpha}^{k\,\mathsf{T}}\nabla g(\boldsymbol{\alpha}^k) \end{aligned}$$

1. Estimate the dual objective function using a linear approximation ∇g.
2. Dual objective value at $\boldsymbol{\alpha}^k$ is computed by $\boldsymbol{\alpha}^{k\,\mathsf{T}}\nabla g(\boldsymbol{\alpha}^k)$.
3. Primal objective value is estimate by $C^{\mathsf{T}}\nabla g(\boldsymbol{\alpha}^k)$.

Experimental results - Objective value

- Compare update with the best direction v.s. update with multiple directions
- Number of spanning trees $|T| = \{5, 10, 20\}$.
- Each spanning tree outputs top $\kappa = 1$ best direction.



Experimental results - Objective value

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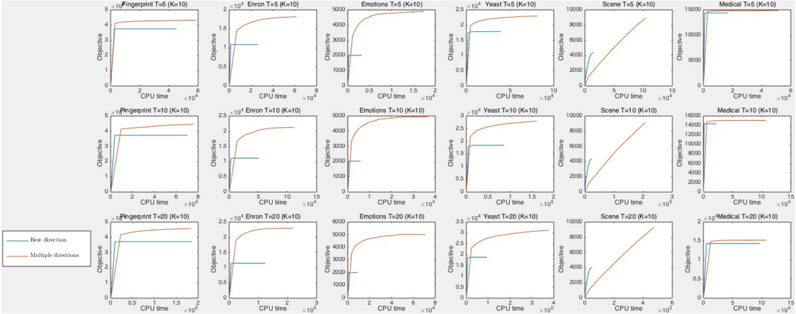

Experimental results - Duality gap

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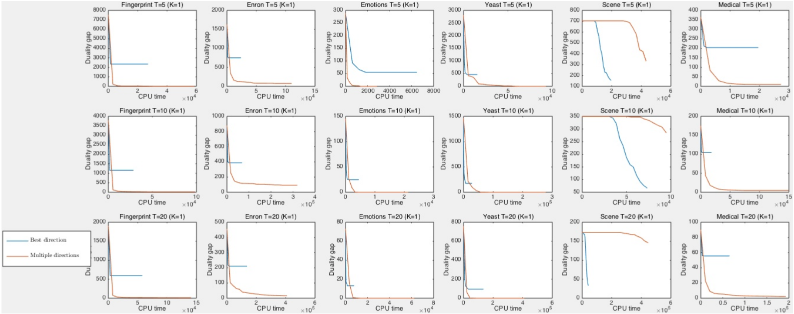

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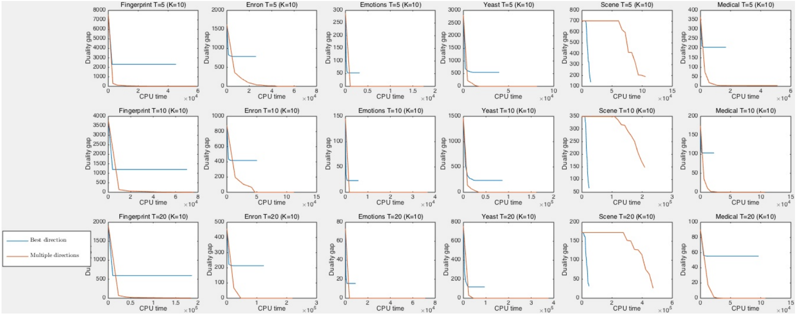
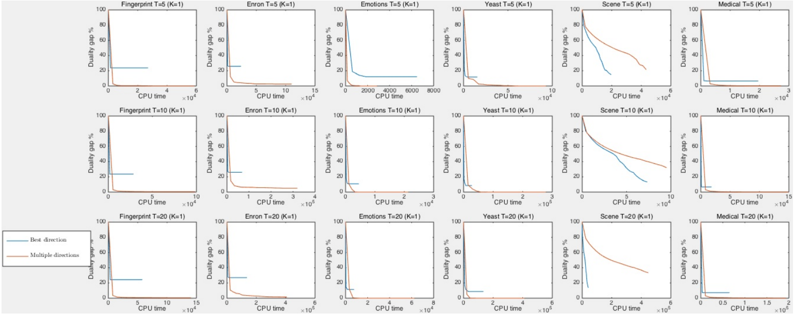


Experimental results - Relative duality gap

- Compare update with the best direction v.s. update with multiple directions
- Number of spanning trees $|T| = \{5, 10, 20\}$.
- Each spanning tree outputs top $\kappa = 1$ best direction.



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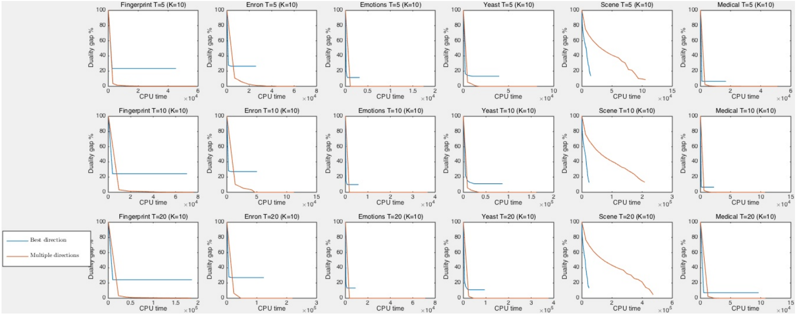

Experimental results - Hamming loss training

- Compare update with the best direction v.s. update with multiple directions
- Number of spanning trees $|T| = \{5, 10, 20\}$.
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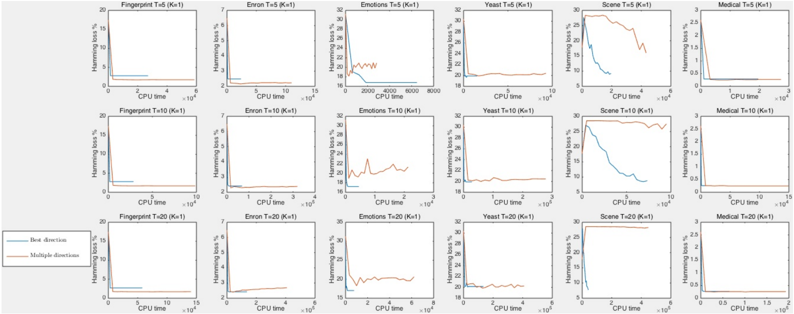

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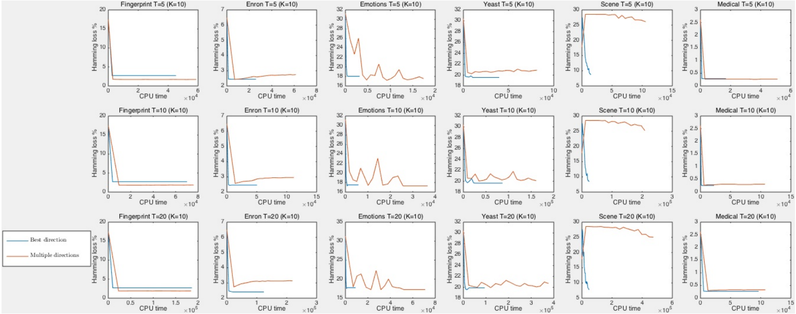
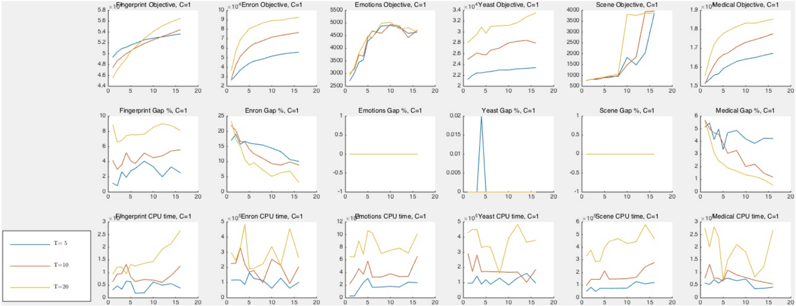


Experimental results

- Multiple update.
- Number of spanning trees $|T| = \{5, 10, 20\}$.
- Each spanning tree outputs $\kappa = \{1, \cdots, 16\}$ best directions.
- Objective value, duality gap, CPU time versus iteration.



Experimental results

- Multiple update.
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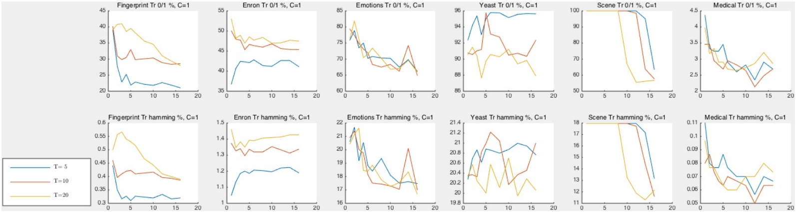
- Training 0/1 loss, hamming loss versus iteration.



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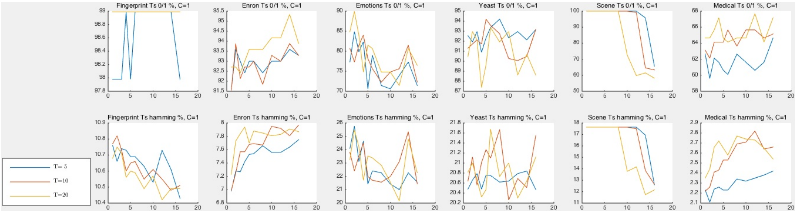

Conclusions

- *Pros:*
  1. Achieves much better objectives, duality gaps.
  2. The quality of the optimization increases as more update directions are used.
  3. Improves training and test error in many datasets.
- *Cons:*
  1. Consumes more CPU times.
  2. The improvements are not dramatic compare to the *best update*.