



# Diverse Particle Selection for High-Dimensional Inference in Graphical Models



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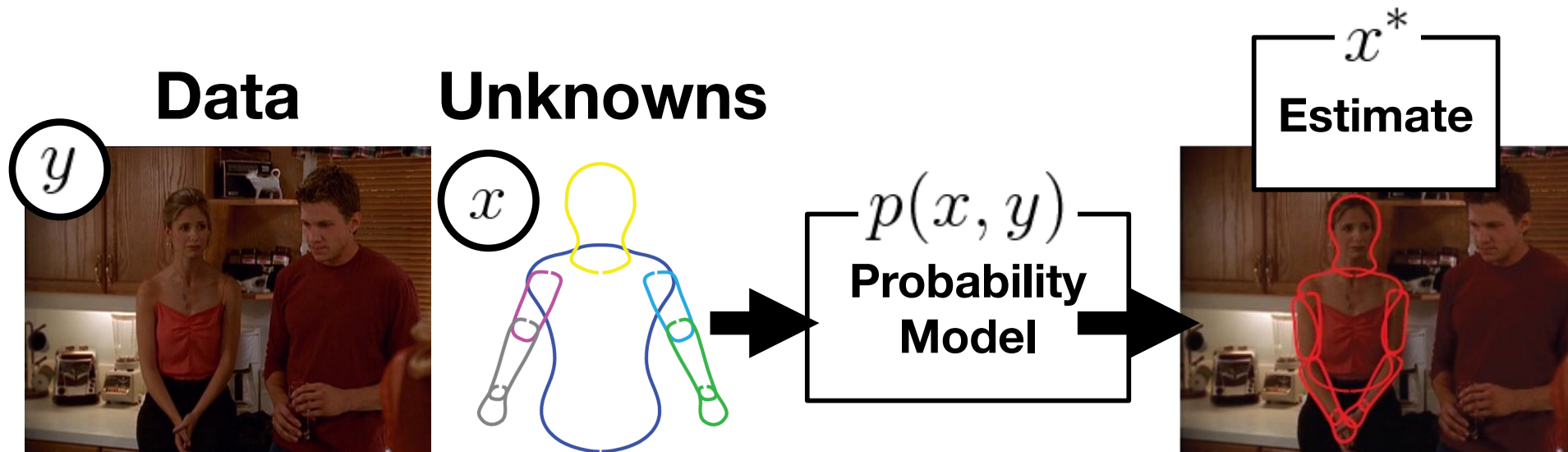
## Collaborators:

- *Particle Max-Product*: Jason Pacheco, MIT
- *Human Pose*: Silvia Zuffi & Michael Black, MPI Tubingen

*Related papers at ICML 2014 & ICML 2015*



# High-Dimensional Inference



**Discrete  
Unknowns**

Efficient inference based on *combinatorial optimization*

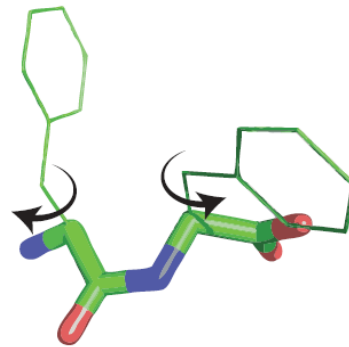
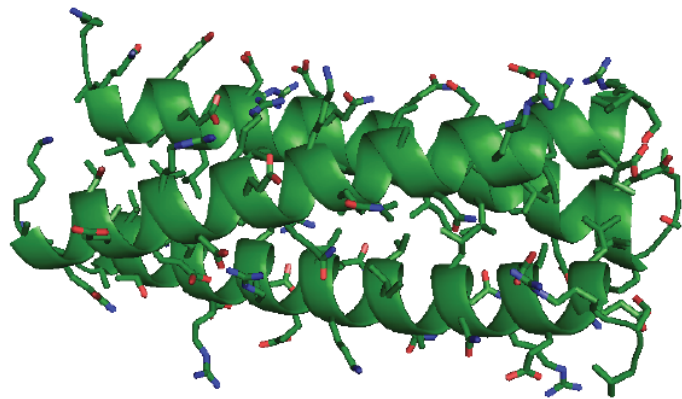
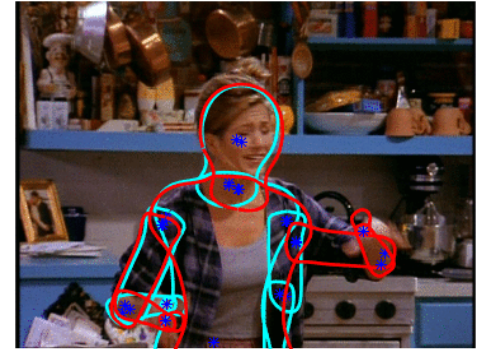
**Continuous  
Unknowns**

Unless we make unrealistic model approximations, *no efficient general solutions. Standard gradient-based optimization is ineffective.*

# Continuous Inference Problems

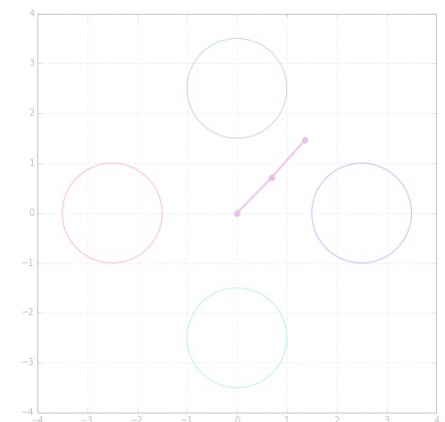
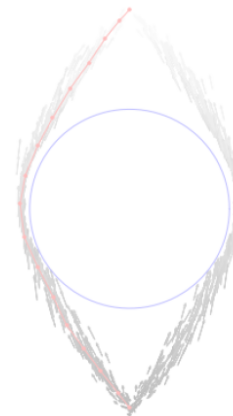


Human pose estimation & tracking

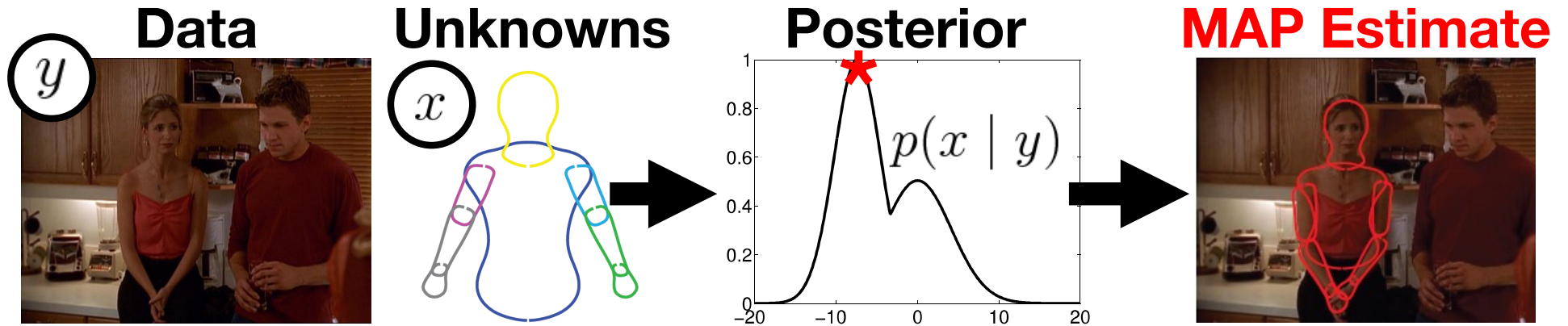


Protein structure & side chain prediction

Robot motion & vehicle path planning



# Maximum a Posteriori (MAP)

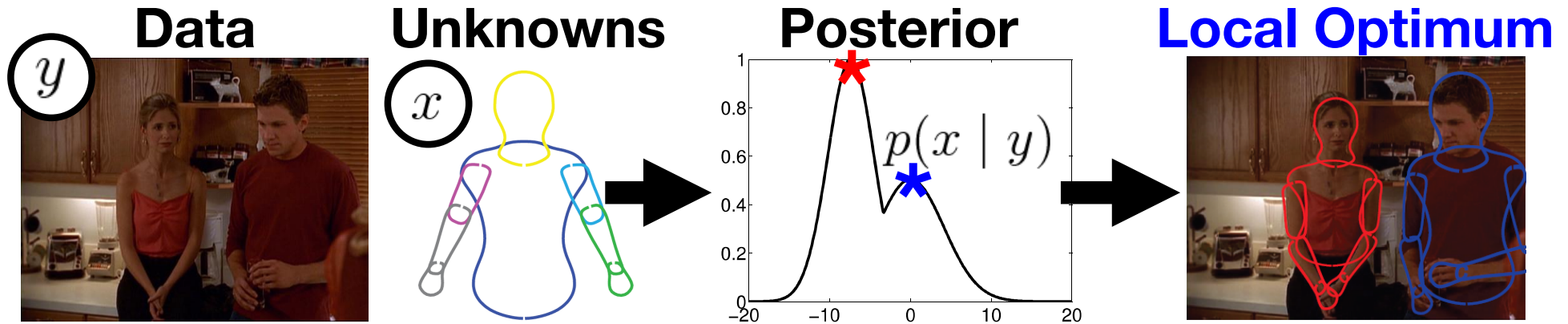


Posterior often intractable and multimodal complicating **exact MAP** inference:

$$x^* = \operatorname{argmax}_x p(x | y)$$



# Maximum a Posteriori (MAP)



Posterior often intractable and multimodal complicating **exact MAP** inference:

$$x^* = \operatorname{argmax}_x p(x | y)$$

**Local optima** can be useful when models are inaccurate or data are noisy.

# Goal

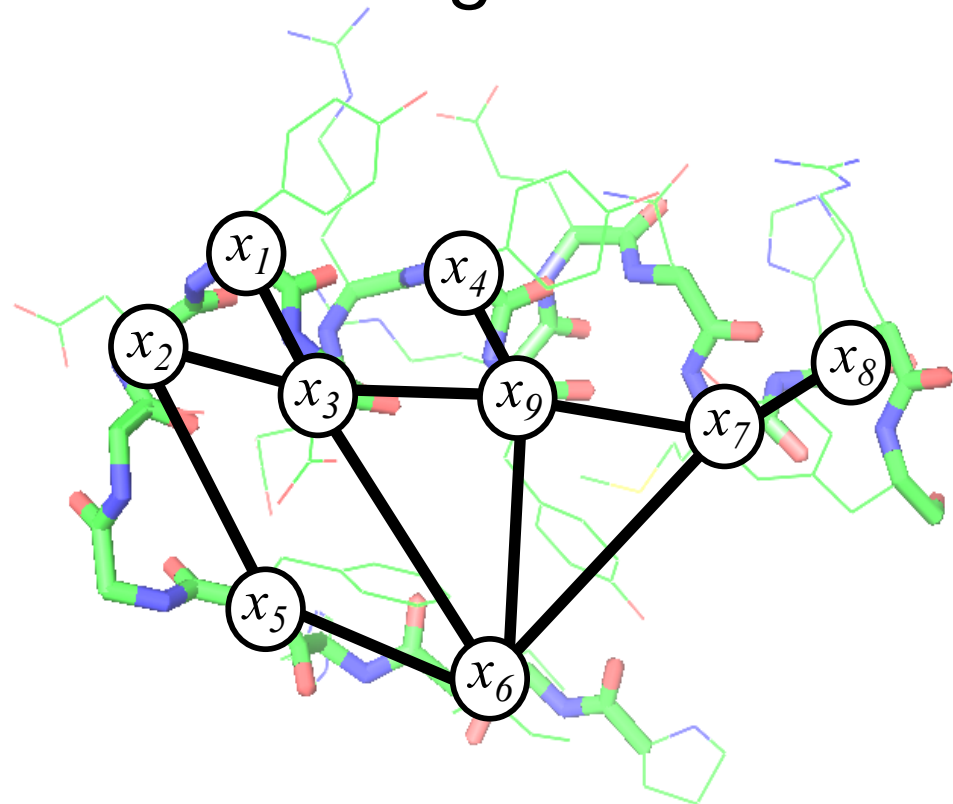
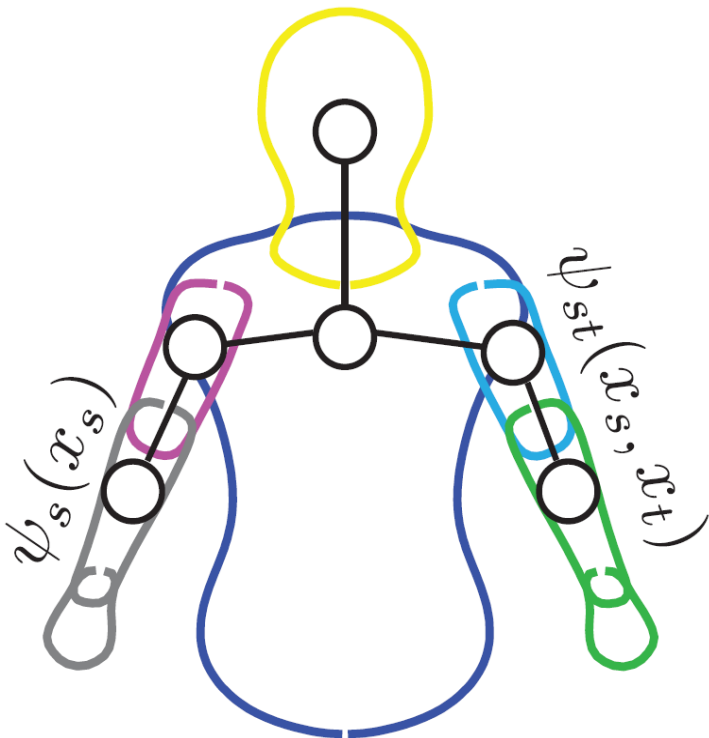
Develop **maximum a posteriori (MAP) inference** algorithms for **continuous probability models** that:

- Apply to *any pairwise graphical model*, even if model is complex (highly non-Gaussian)
- Are *black-box* (no gradients required)
- Will *reliably* infer multiple local optima

# Pairwise Graphical Models

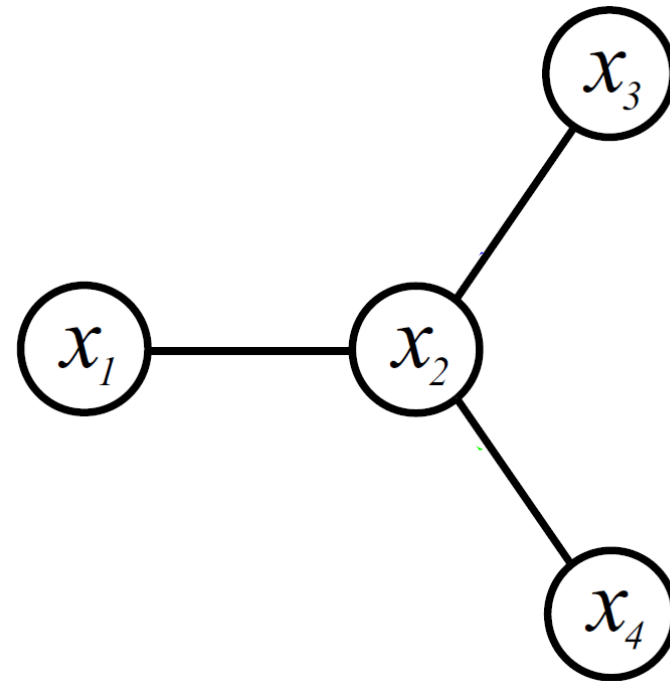
$$p(x) \propto \prod_{s \in \mathcal{V}} \psi_s(x_s) \prod_{(s,t) \in \mathcal{E}} \psi_{st}(x_s, x_t) \quad x_s \in \mathbb{R}^d$$

- Nodes are continuous random variables
- Potentials encode statistical relationships
- Edges indicate direct, pairwise energetic interactions



# Message Passing on Trees

Global MAP inference decomposes into local computations via graph structure...



$$\begin{aligned} \max_x p(x) &\propto \max_x \psi_{12}(x_1, x_2) \psi_{23}(x_2, x_3) \psi_{24}(x_2, x_4) \\ &= \max_{x_1} \max_{x_2} \psi_{12}(x_1, x_2) \underbrace{\left[ \max_{x_3} \psi_{23}(x_2, x_3) \right]}_{m_{32}(x_2)} \underbrace{\left[ \max_{x_4} \psi_{24}(x_2, x_4) \right]}_{m_{42}(x_2)} \\ &\quad \underbrace{\hspace{15em}}_{m_{21}(x_1)} \end{aligned}$$



# Max-Product Belief Propagation

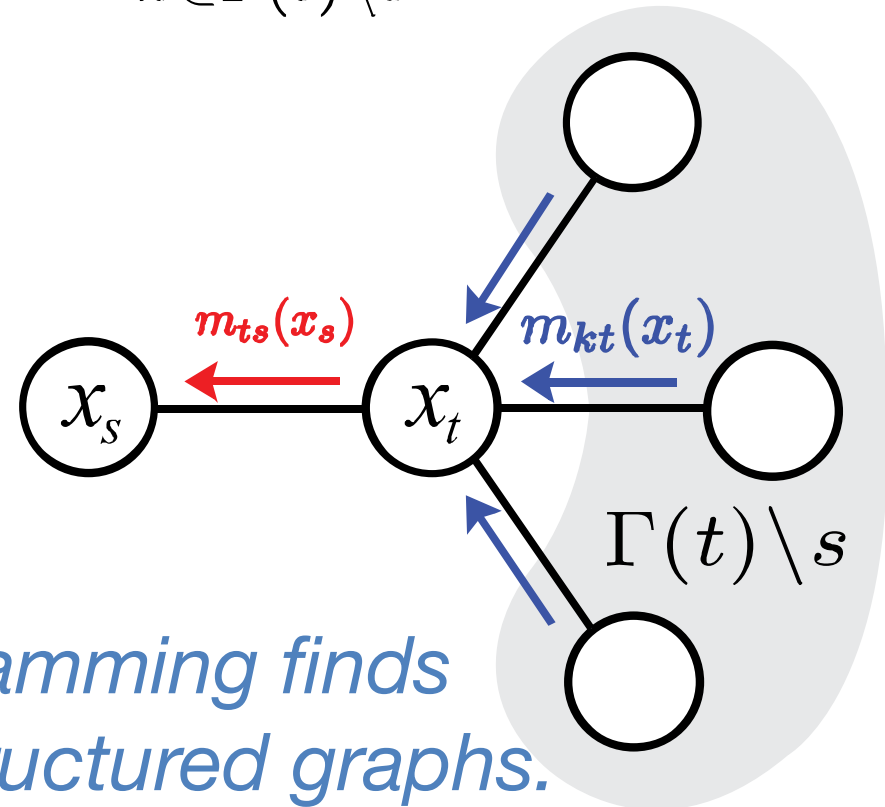
*Finding max-marginals via message-passing*

$$q_s(x_s) = \max_{x_{t \neq s}} p(x_s, x_{t \neq s}) \propto \psi_s(x_s) \prod_{t \in \Gamma(s)} m_{ts}(x_s)$$

$$m_{ts}(x_s) = \max_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t) \prod_{k \in \Gamma(t) \setminus s} m_{kt}(x_t)$$

Why max-marginals?

- Directly encode global MAP
- Other modes important: models approximate, data uncertain



*Max-product dynamic programming finds exact max-marginals on tree-structured graphs.*





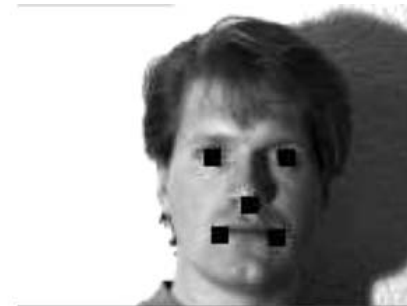
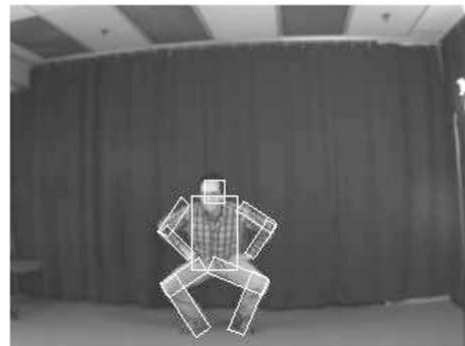
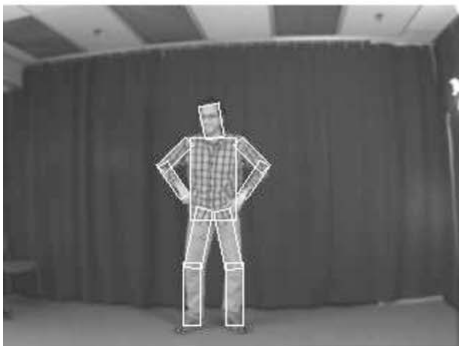
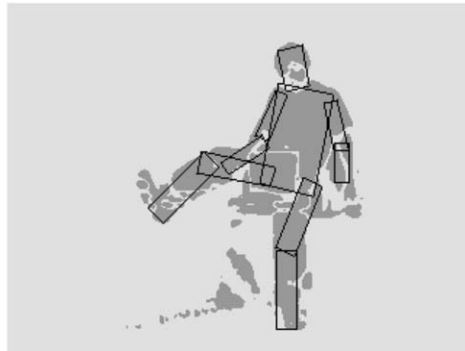
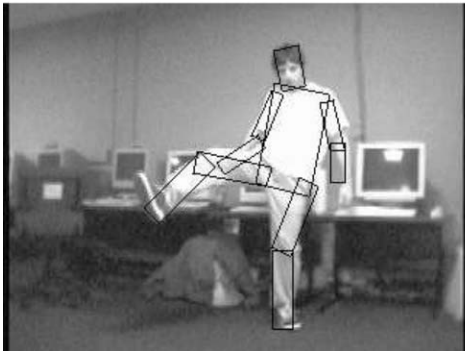
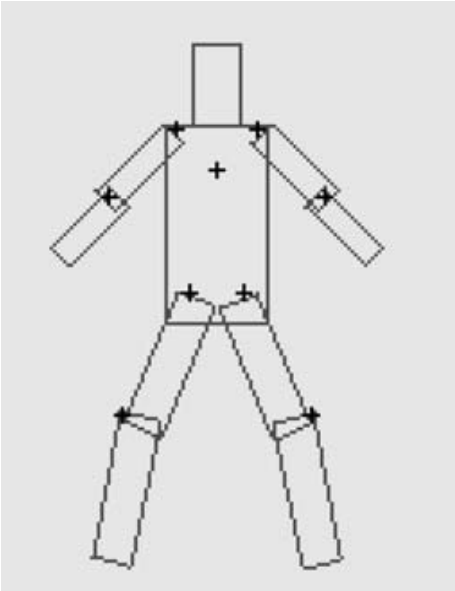
# Poses & Discrete Probabilities

*Felzenszwalb & Huttenlocher, 2005*

*Localize object via  
MAP estimate in  
pairwise MRF  
with rigid geometry.*

$$p(L | \theta) = \frac{\prod_{(v_i, v_j) \in E} p(l_i, l_j | \theta)}{\prod_{v_i \in V} p(l_i | \theta)^{\deg v_i - 1}}$$

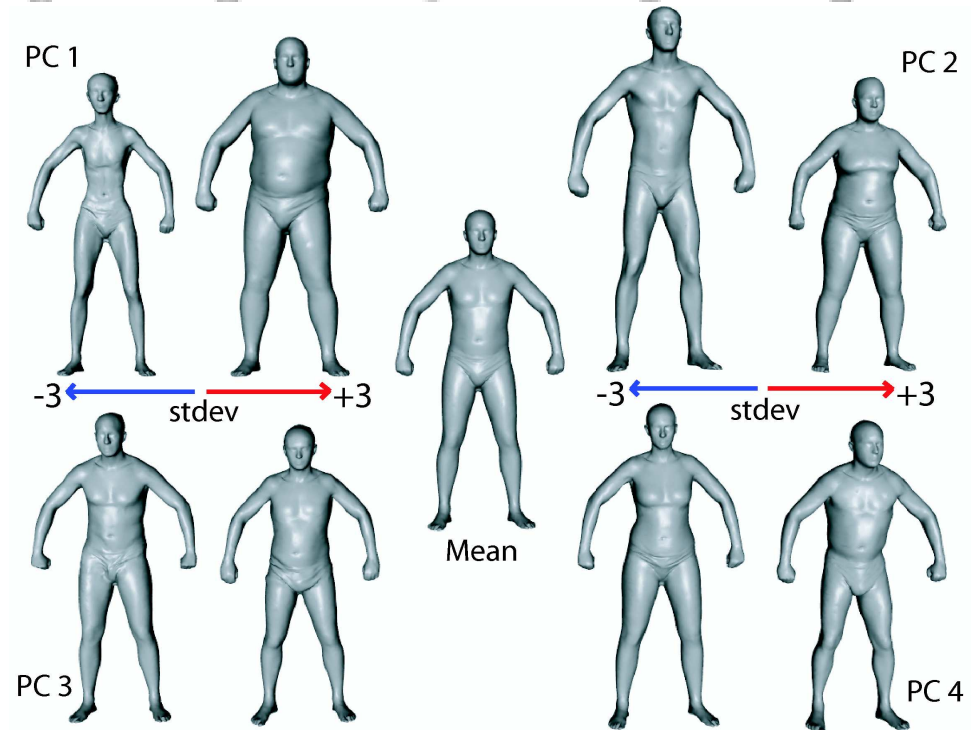
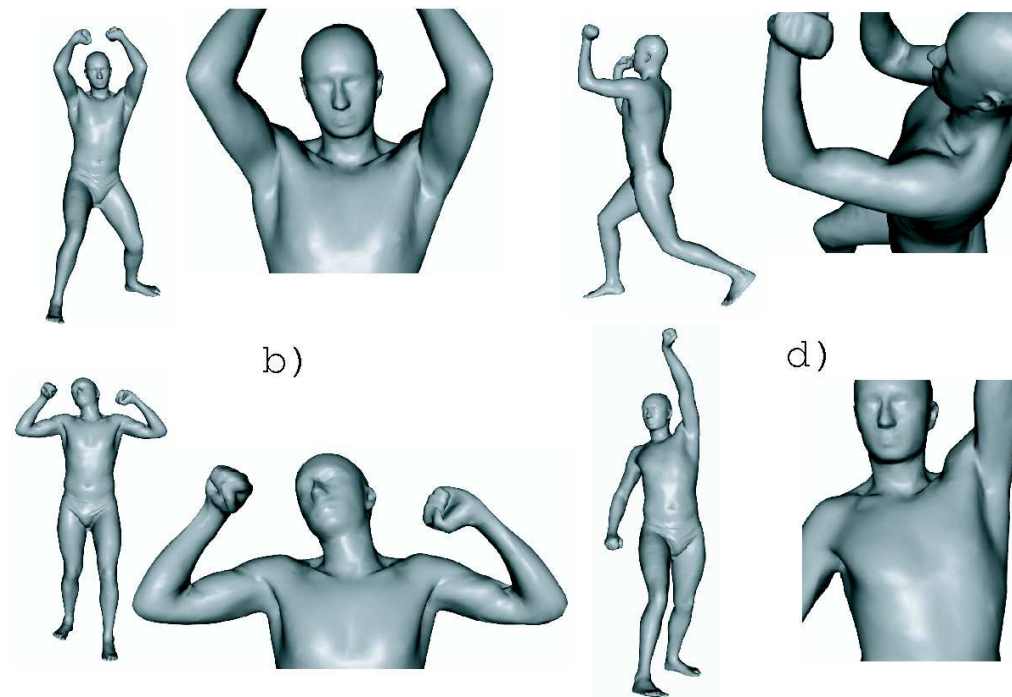
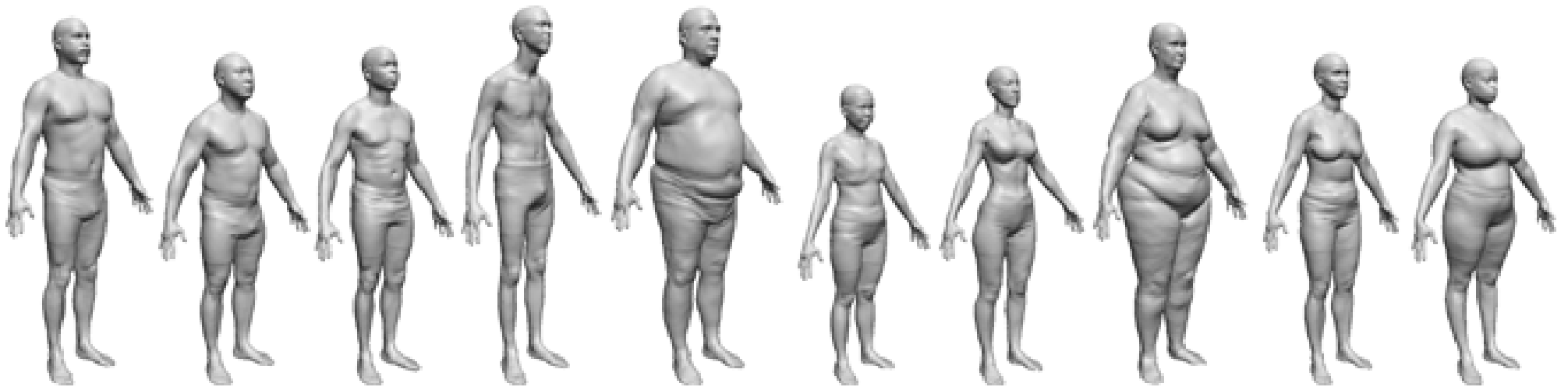
$$p(I | L, \theta) = p(I | L, u) \propto \prod_{i=1}^n p(I | l_i, u_i).$$





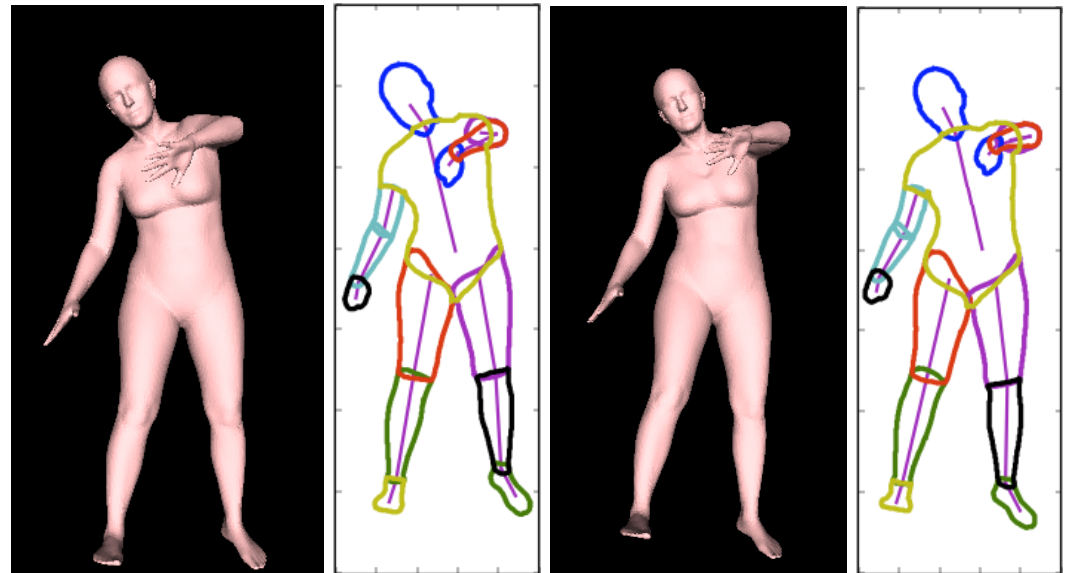
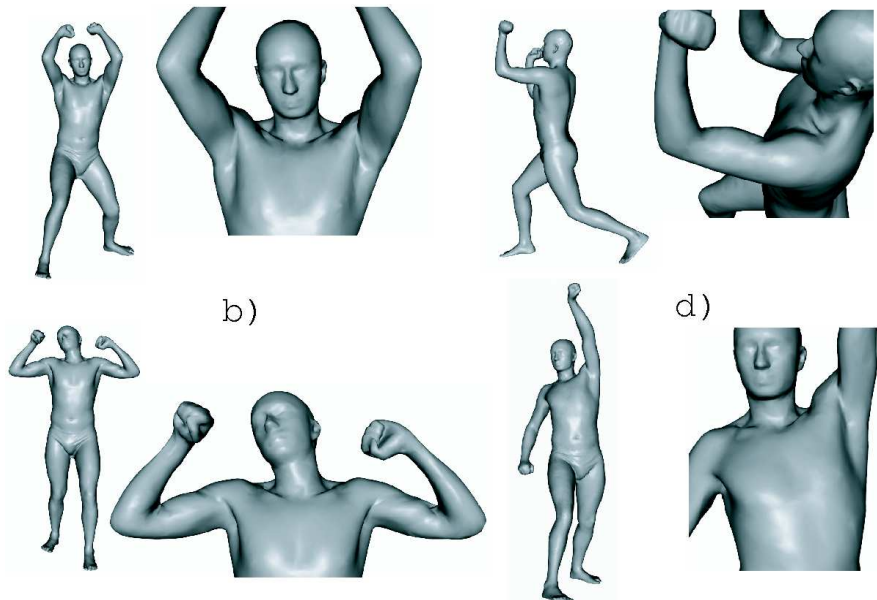
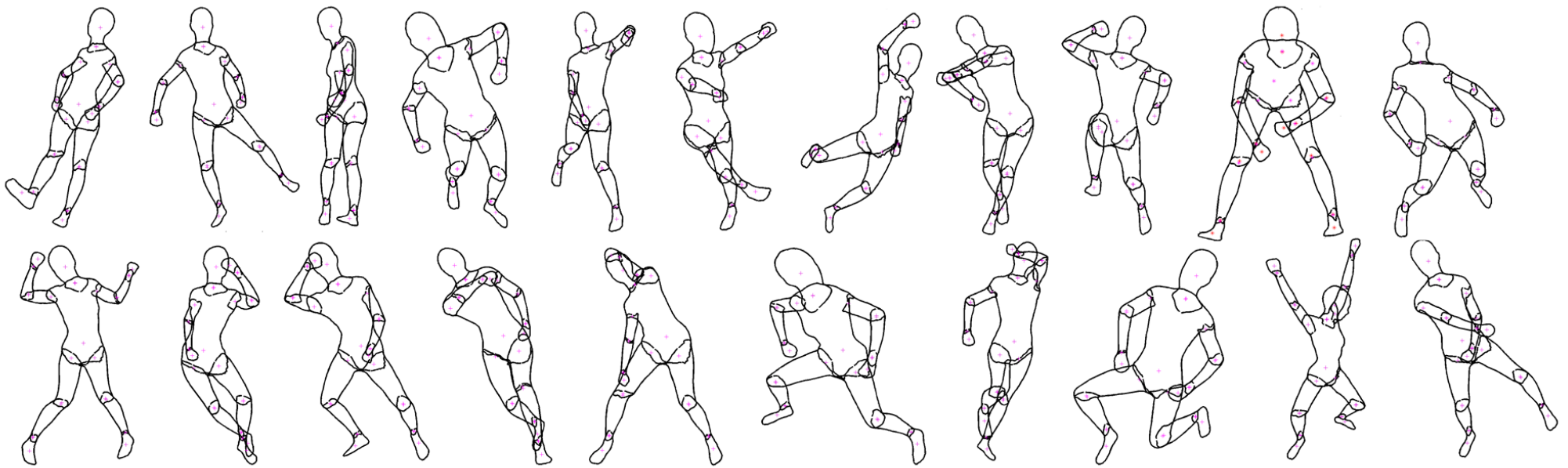
# SCAPE

*Shape Completion and Animation of People, Anguelov et al. 2004*



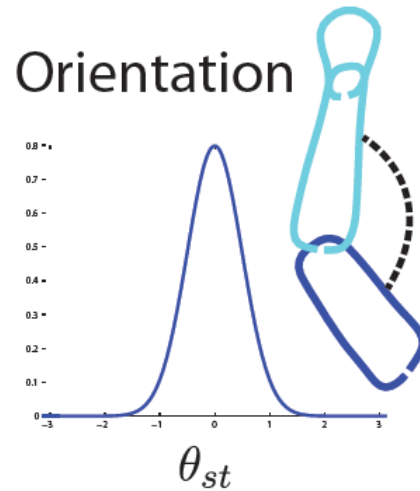
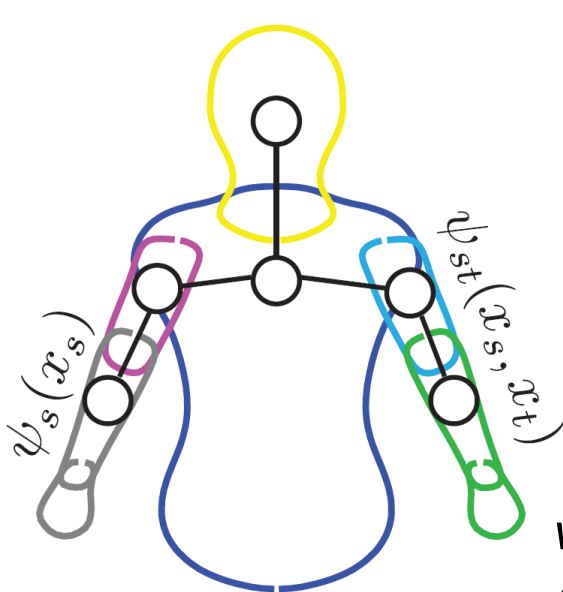
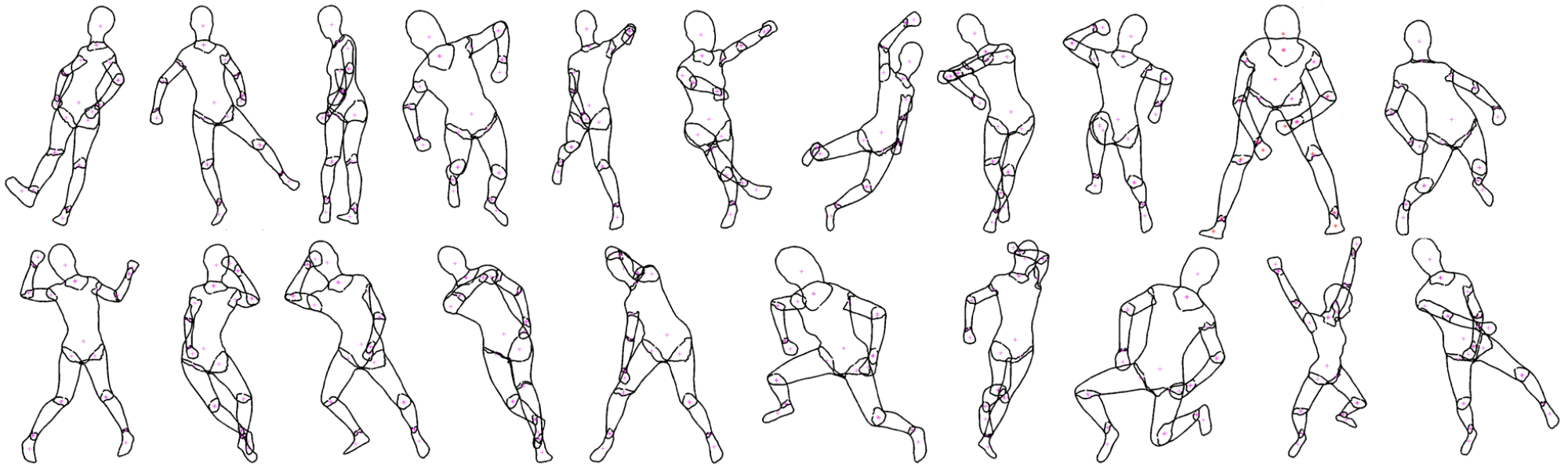
# Deformable Structures

*Zuffi, Freifeld, & Black, CVPR 2012*

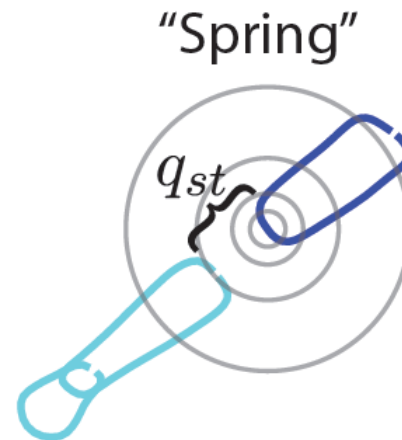


# Deformable Structures

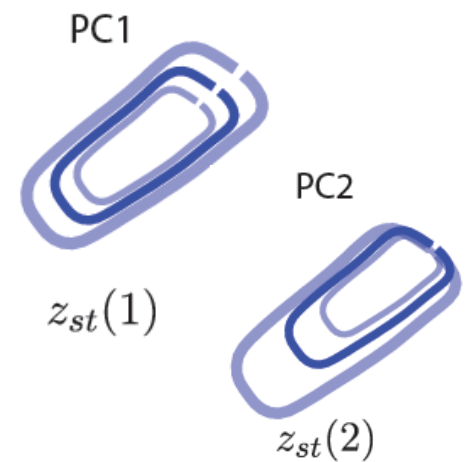
Zuffi, Freifeld, & Black, CVPR 2012



*von Mises distribution on relative orientation*



*Gaussian distribution on relative position*

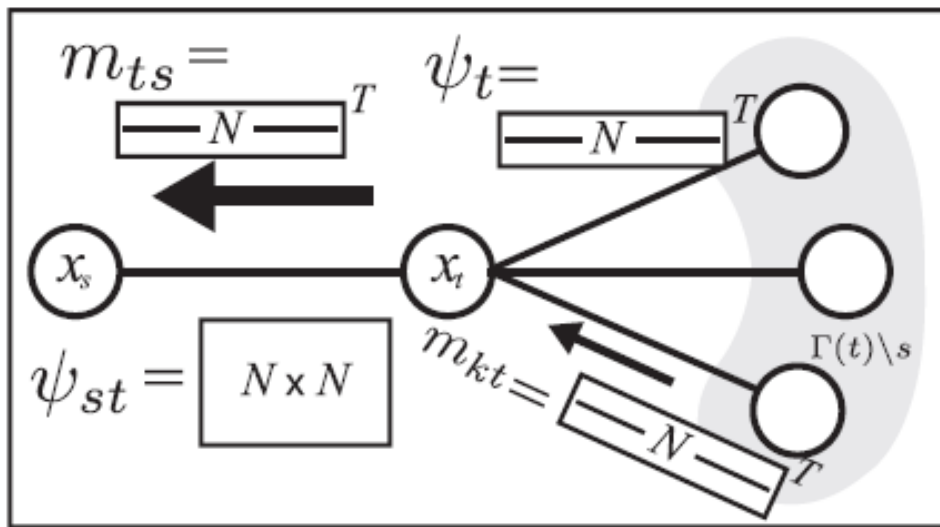


*PCA model of part shape*

# Max-Product Belief Propagation

## Discrete

$$x \in \{1, \dots, N\}^D$$



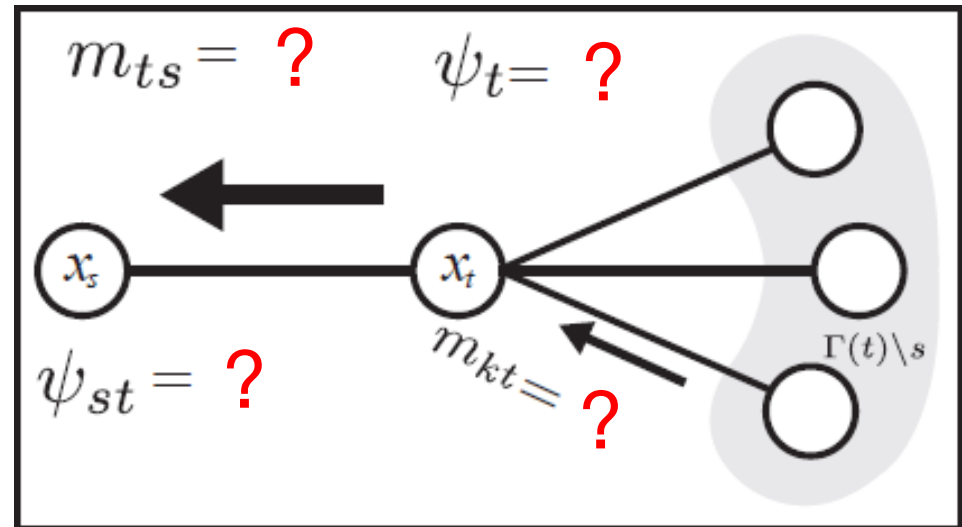
Message Update:

$$m_{ts} = \max_{x_t} \psi_{st} \psi_t \prod m_{kt}$$

Matrix-vector multiplication and discrete maximization.

## Continuous

$$x \in \mathcal{R}^D$$



Message Update:

$$m_{ts}(x_s) = \dots$$

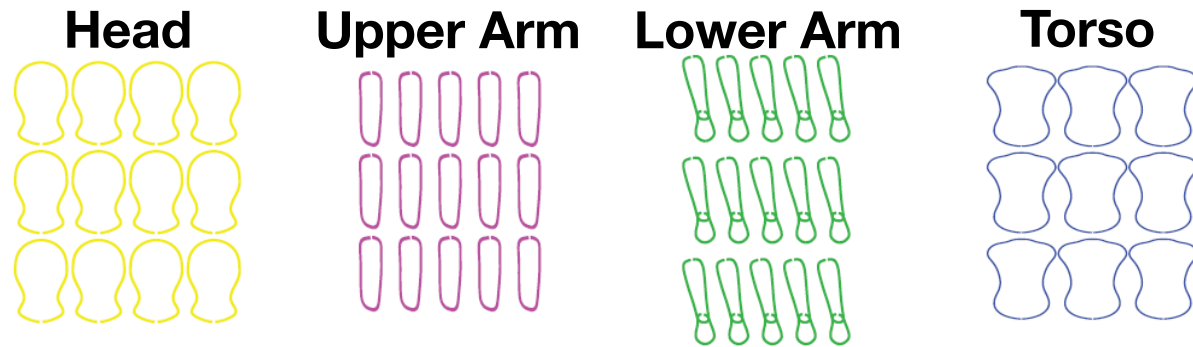
$$\max_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t) \prod m_{kt}(x_t)$$

Messages are functions with no analytic form. Nonlinear optimization.



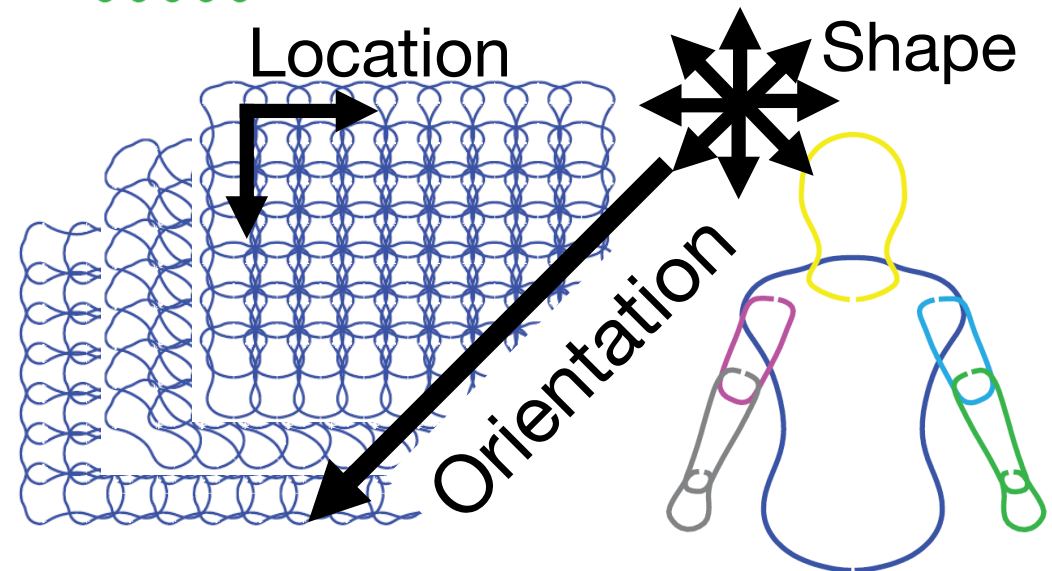
# Regular Discretization Infeasible

Approximate continuous max-product messages over regular *grid* of points?



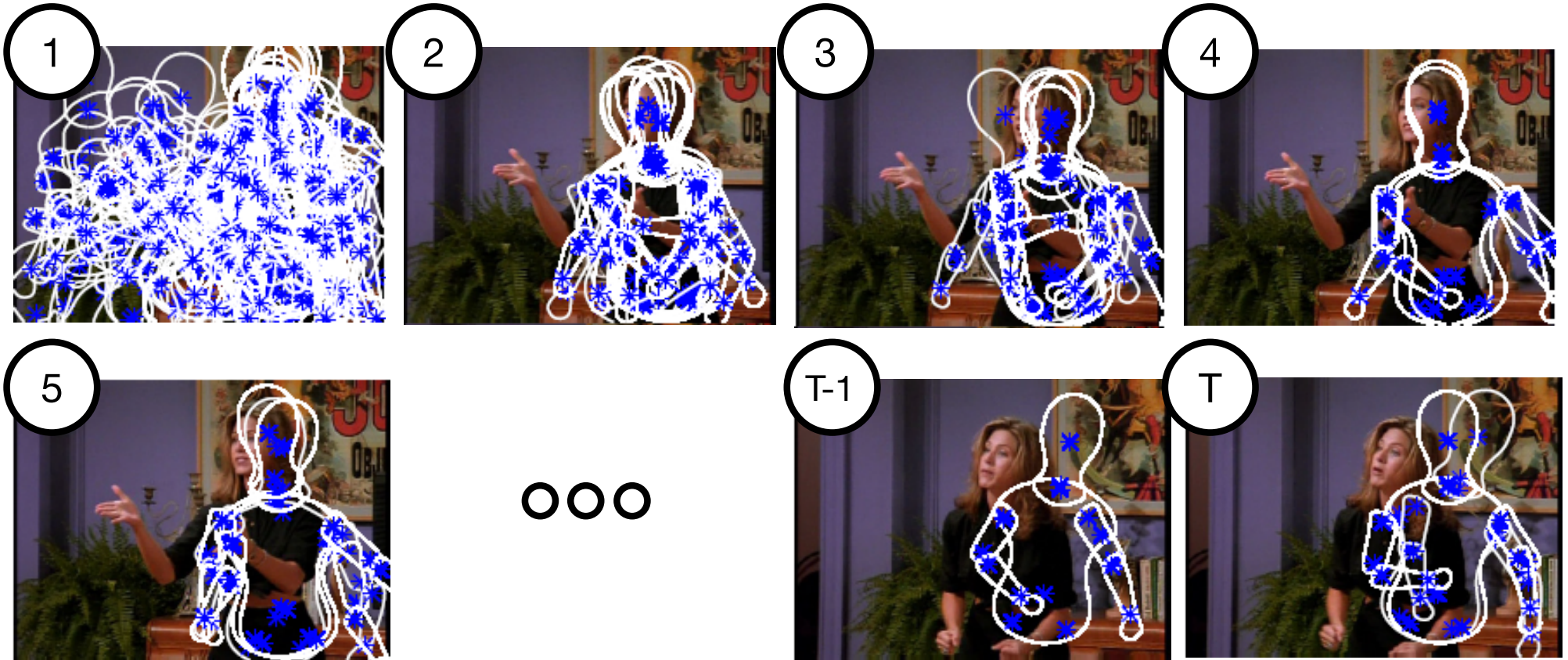
## Example: Torso

- ~10 dimensions.
- 10 grid points per dimension
- 10 Million points!



**Infeasible for high dimensional models.**

# Pose Tracking Particle Filter?



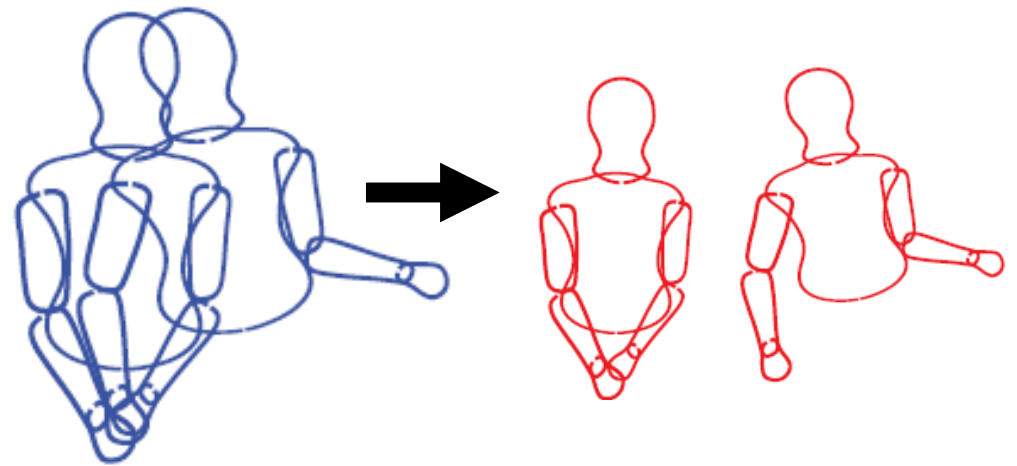
**CONDENSATION** algorithm [Isard & Blake, 1998]

- Particles degenerate over time
- Resampling reduces effective number of particles
- Extension beyond time series models non-trivial

# Particle Representations

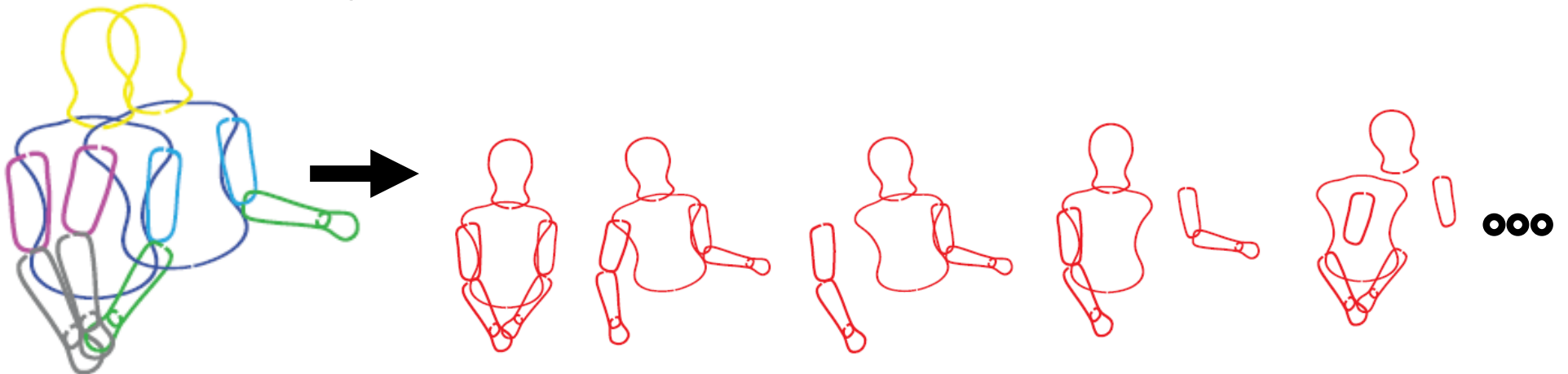
## Particle filter:

- Each particle is a full joint instantiation



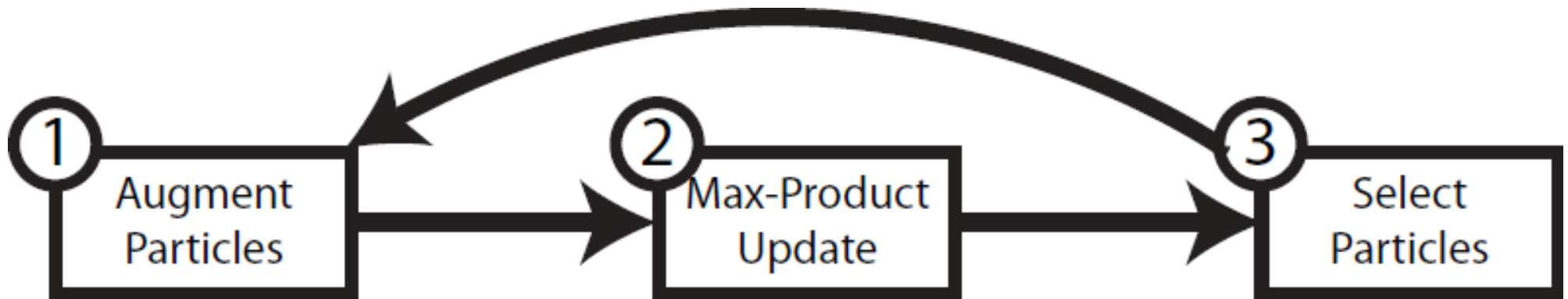
## Max-Product:

- Each particle is a single variable node (part)
- Efficiently enumerates all combinations



# Particle Max-Product (PMP)

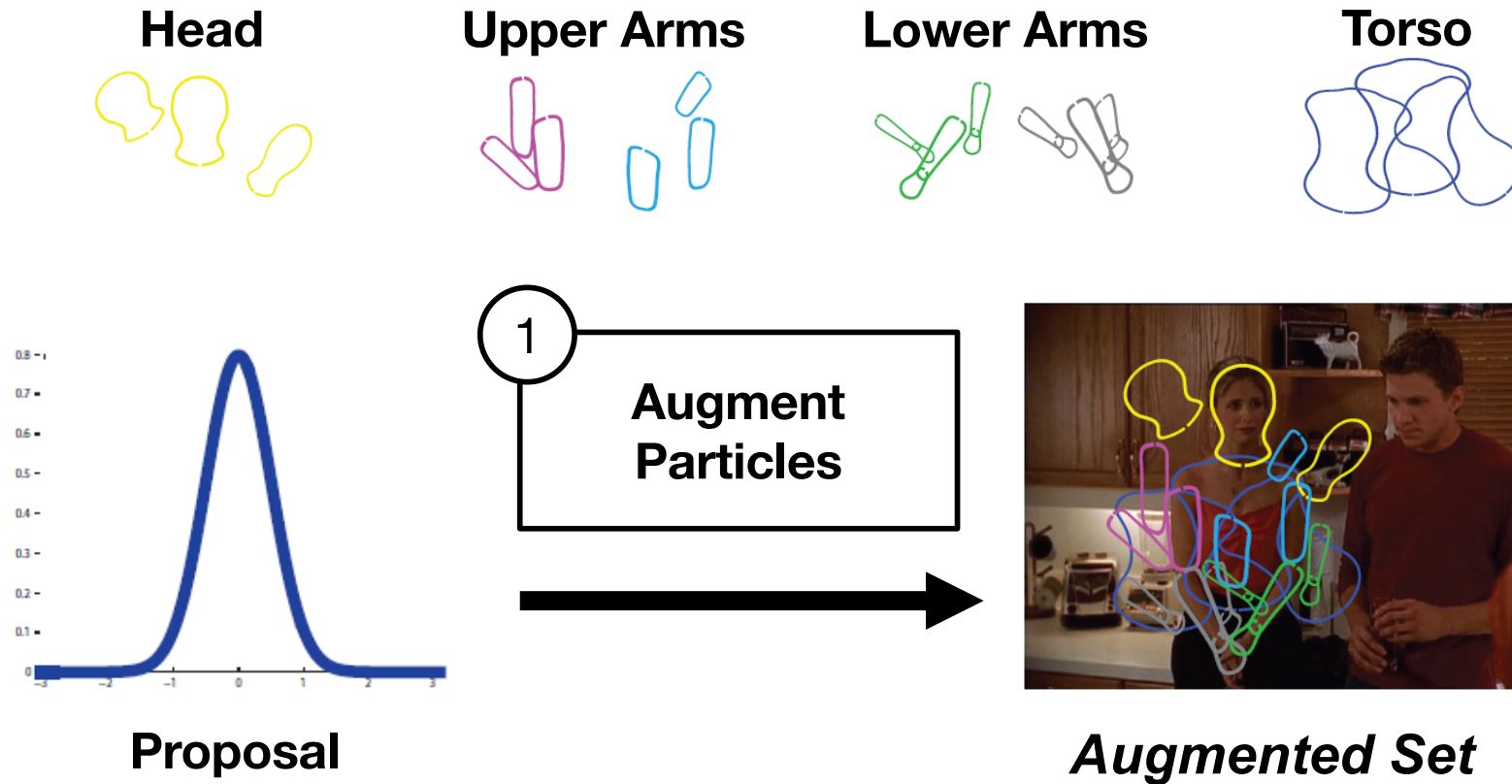
Combine particle filter ideas with max-product more effectively.



Particle approximation of continuous max-product (MP) messages.

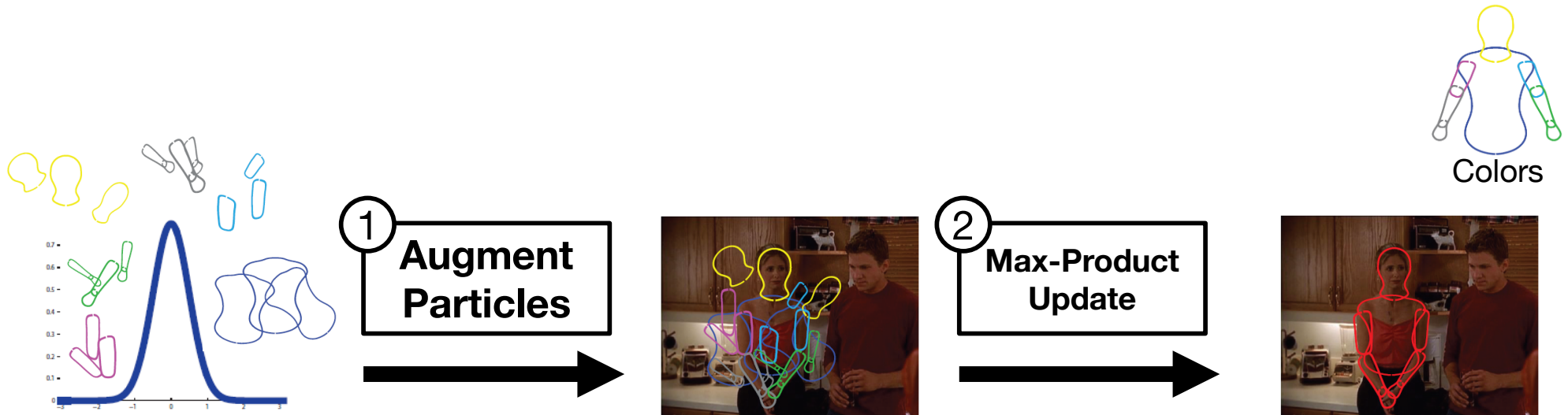


# Particle Max-Product (PMP)



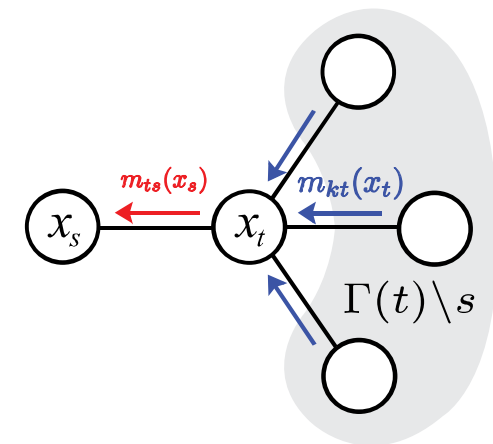
Sample new hypotheses at every node to grow particle set.

# Particle Max-Product (PMP)

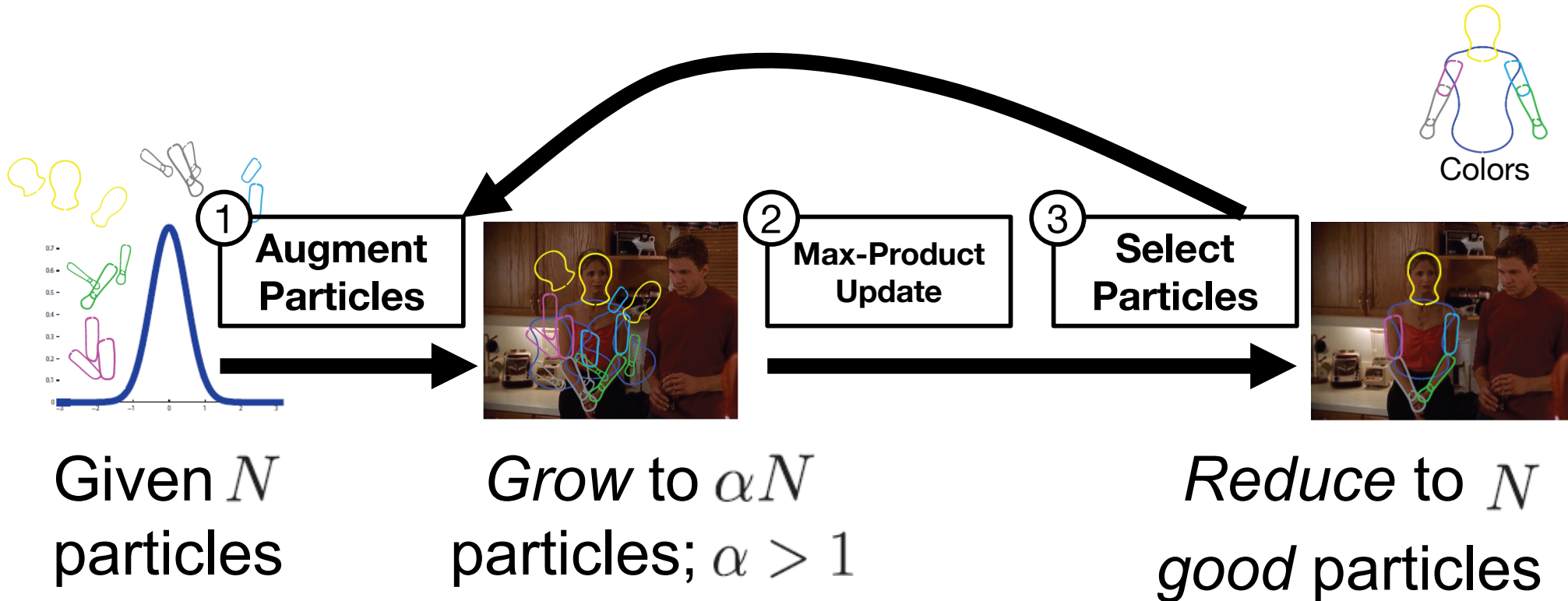


$$m_{ts}(x_s) \propto \max_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t) \prod_{k \in \Gamma(t) \setminus s} m_{kt}(x_t)$$

Update MP messages on augmented particles.



# Particle Max-Product (PMP)



Select subset of *good* particles & repeat

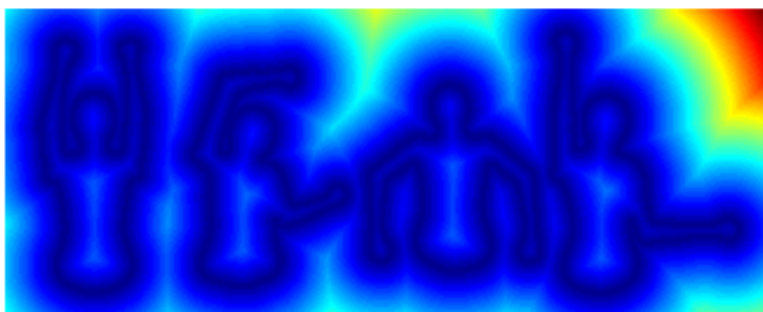
Need a particle selection method...

# Deformable Structures for Silhouettes

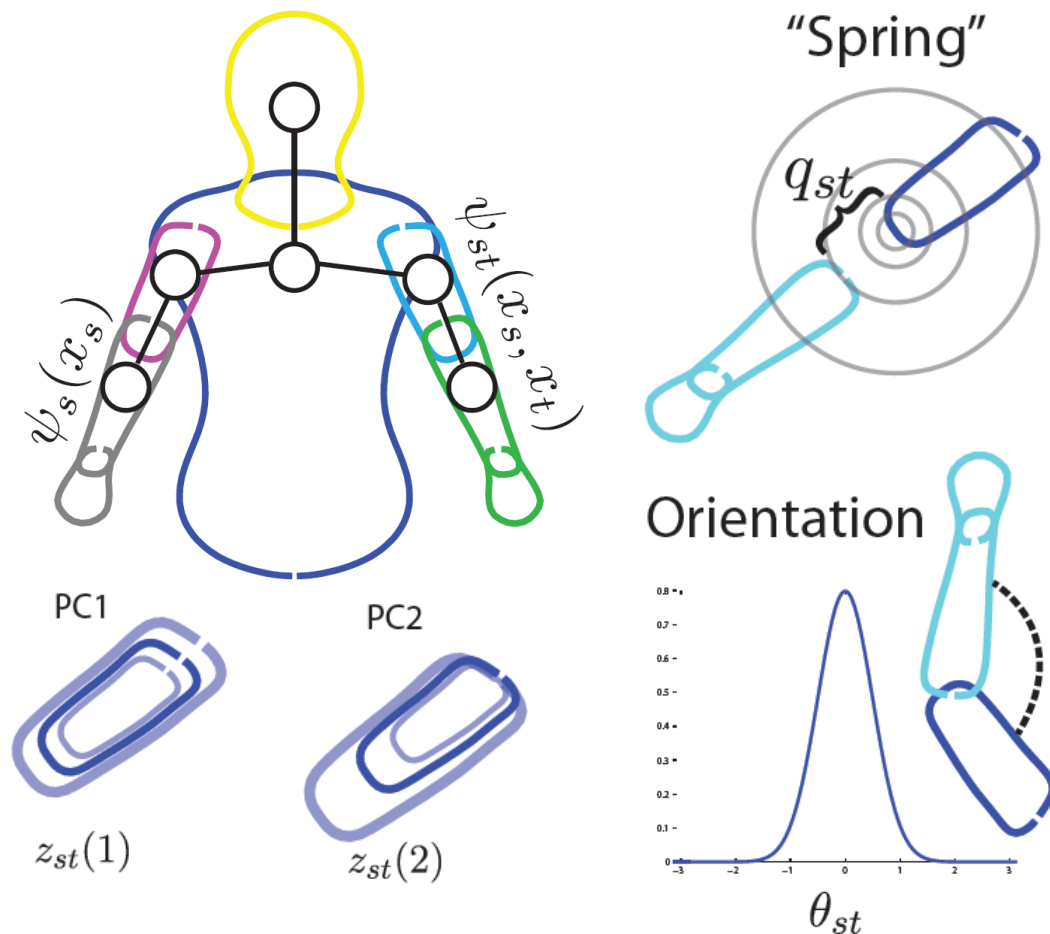
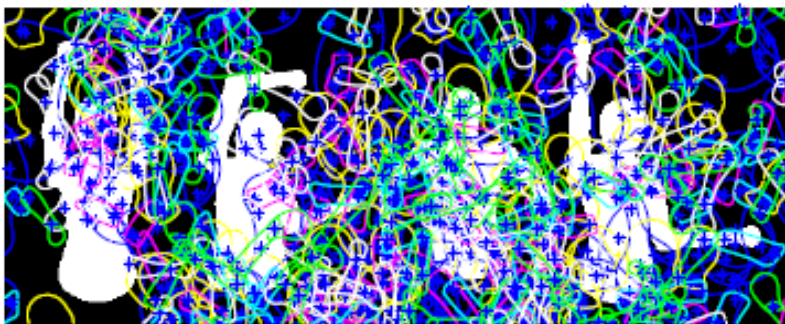
## ICML



Chamfer Distance Likelihood



Random Initialization

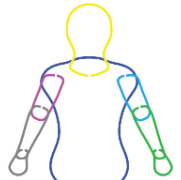


## Inference Goals:

- Accurately localize all 4 people
- Reliably find global MAP (the “M”)

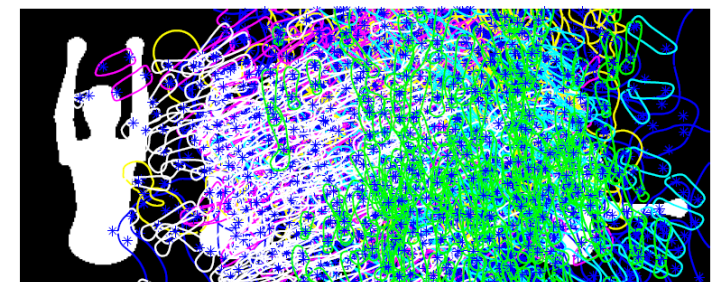
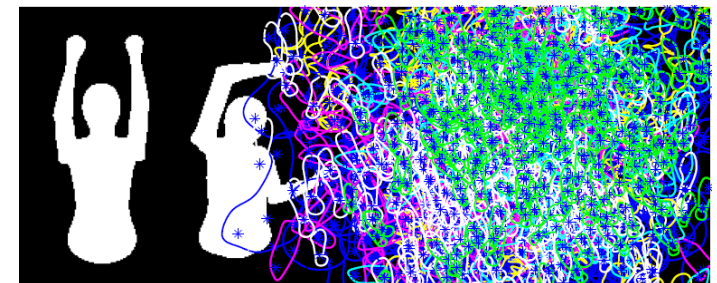
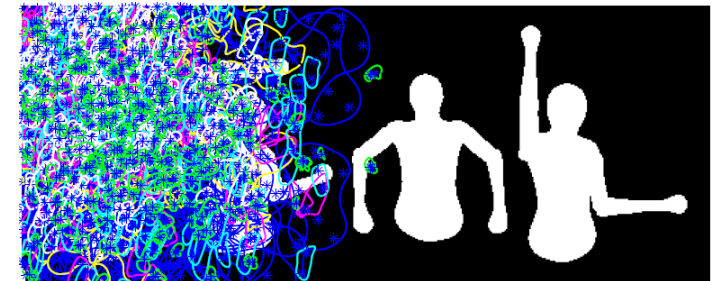
# Greedy Particle Max-Product

*G-PMP: Trinh & McAllester 2009*



Example Runs Colors

- **Select:** Discard all current particles except “MAP”
- **Augment:** Propose new particles by perturbing MAP (Gaussian “random walk”)

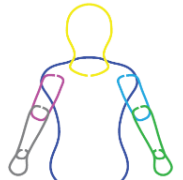
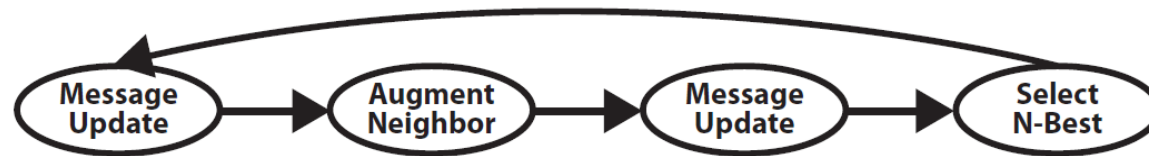


Particles *degenerate* to a single mode. Discovered mode is *very sensitive to initialization*, and is often not the true MAP.



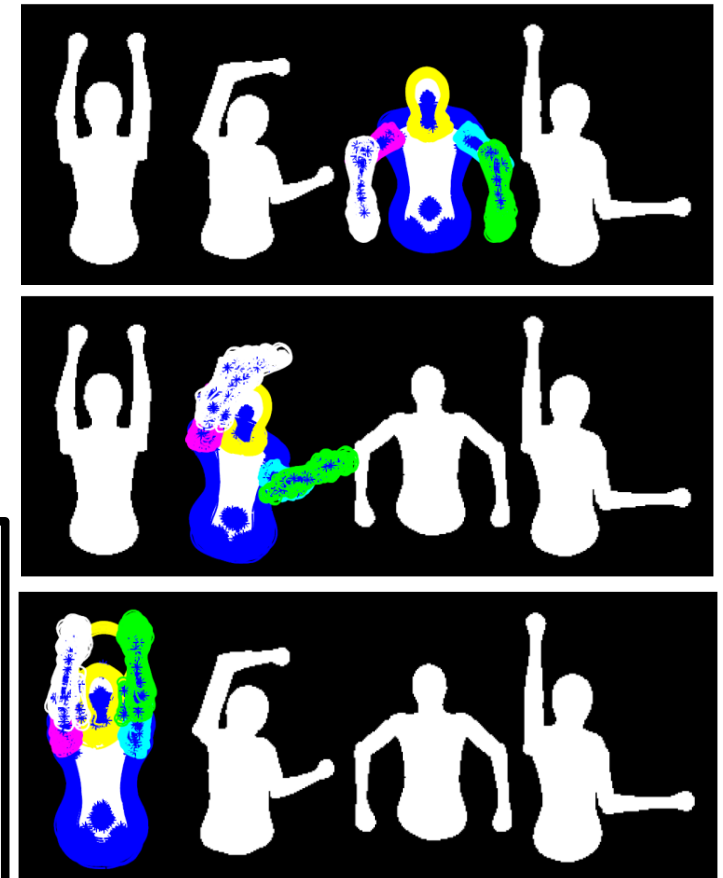
# Top-Mode Particle Max-Product

*T-PMP: Generalization of PatchMatch BP, Besse et al. 2012*



Example Runs Colors

- **Augment:** Propose new particles from neighbors
- **Select:** Sort max-marginals and keep top  $N$  particles

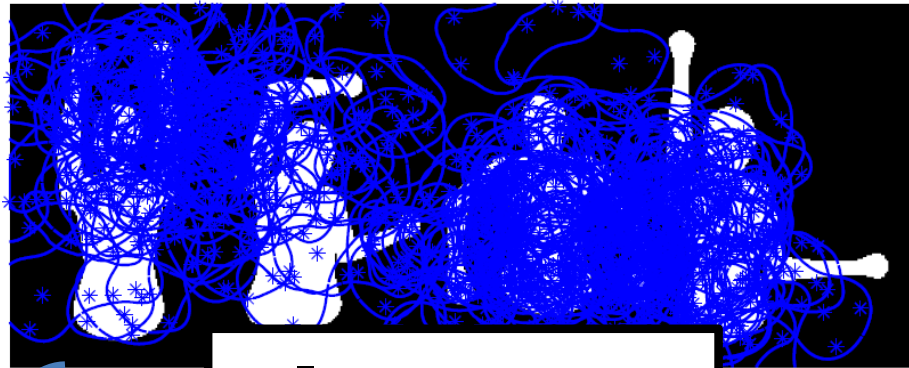


Particles *degenerate* to a single mode. Discovered mode is *sensitive to initialization*, and is often not the true MAP.

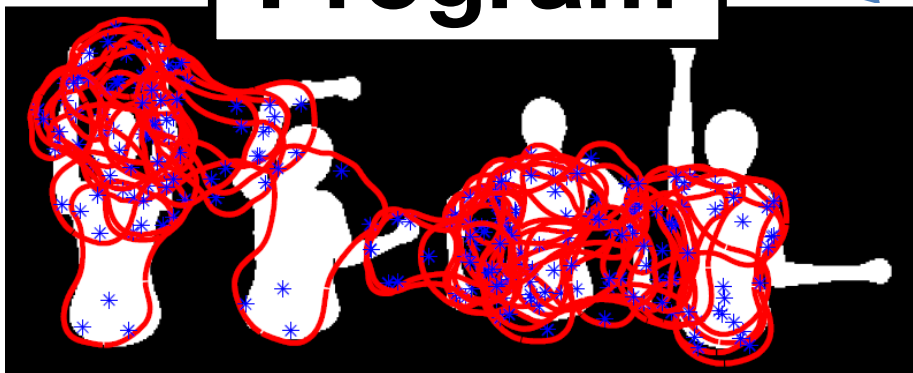
# Diverse Particle Selection

**GOAL:** Maintain *diversity* in particles.

**Initial Particles**

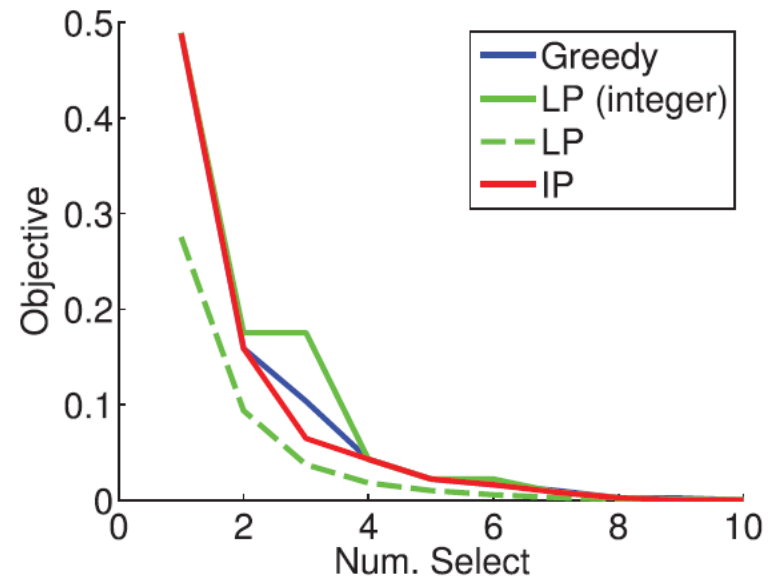


**Integer Program**



**Diverse Selection**

Integer Program (IP)  
solved with efficient  
greedy approximation:

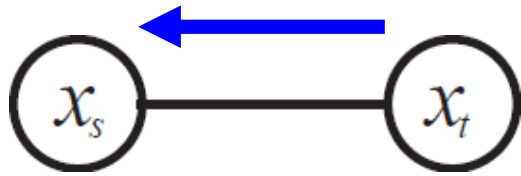


LP : Linear Program relaxation

IP: Optimal solution by brute force

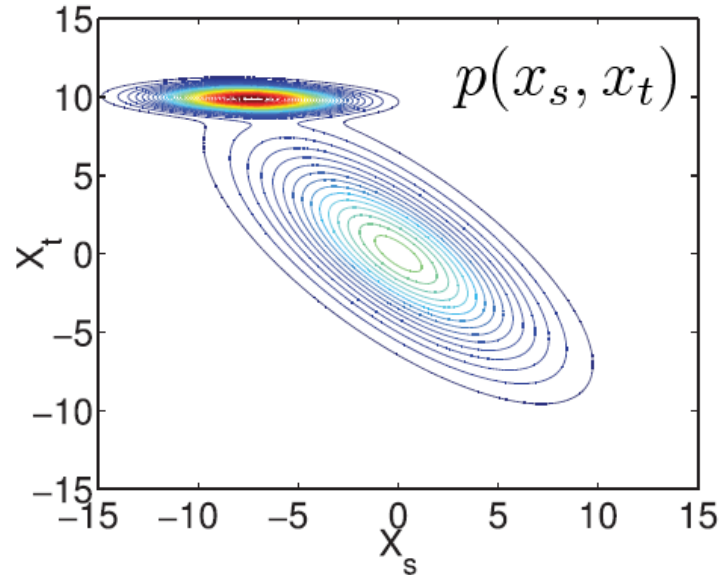
Greedy: Efficient approximation

# Continuous Message

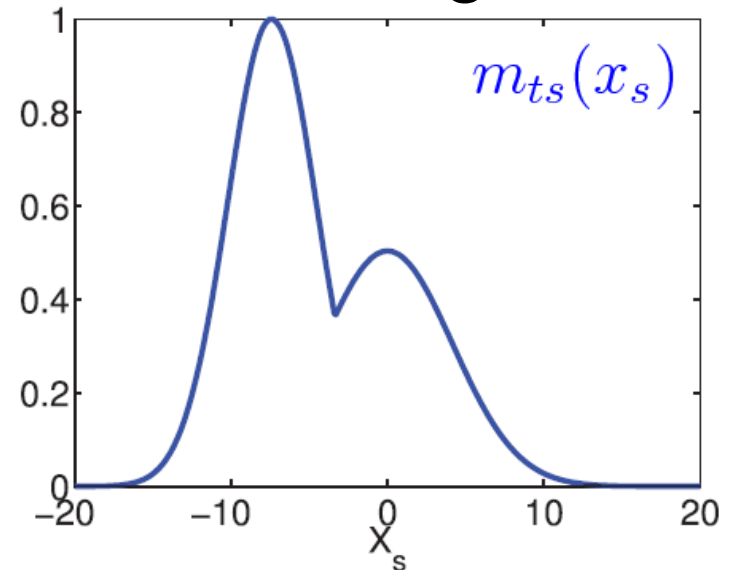


$$m_{ts}(x_s) = \max_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t)$$

## Joint Distribution

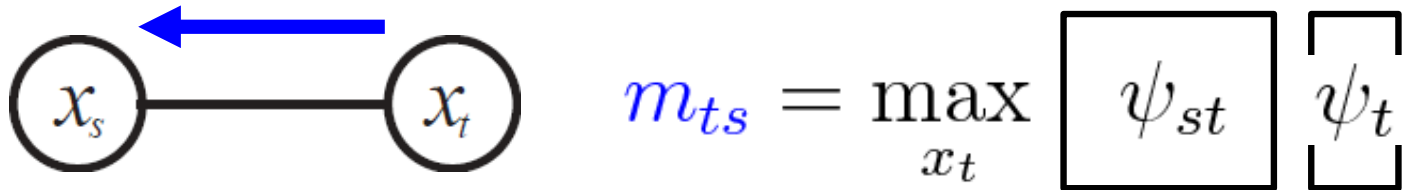


## Message

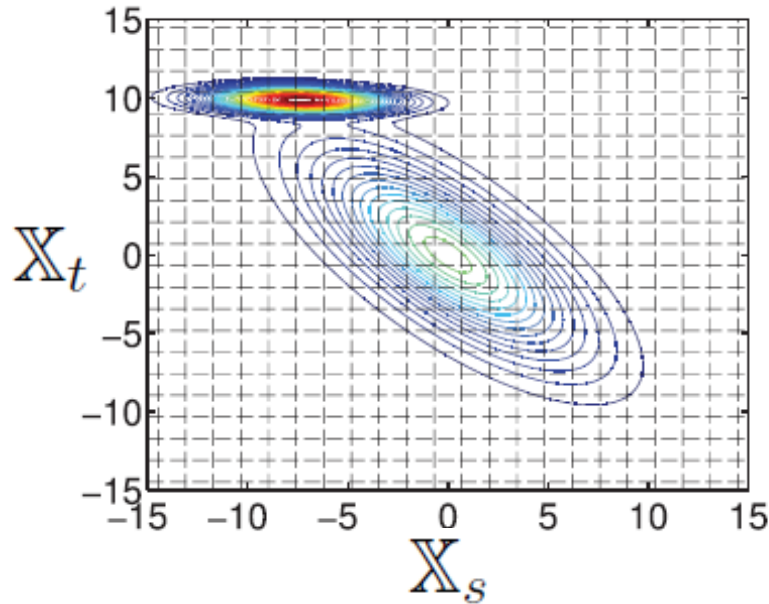


**Model is a mixture of 2 Gaussians.**

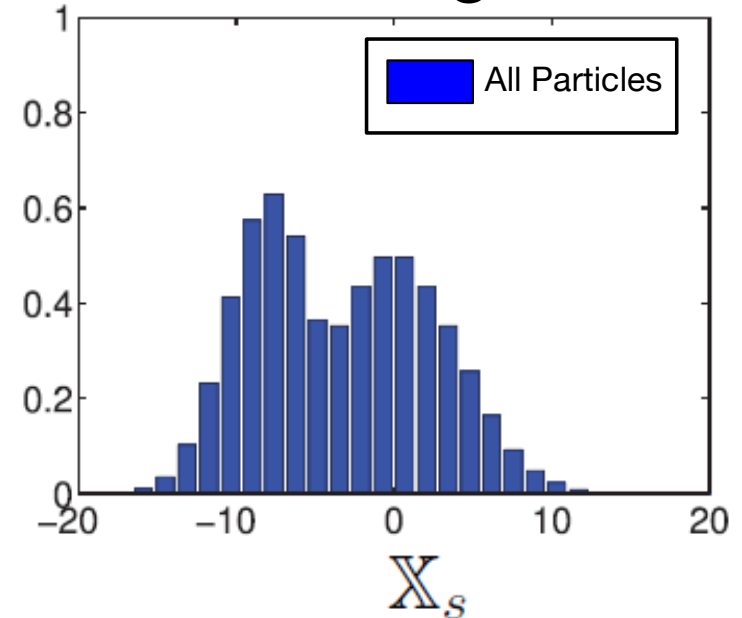
# Discrete Message



Joint Distribution



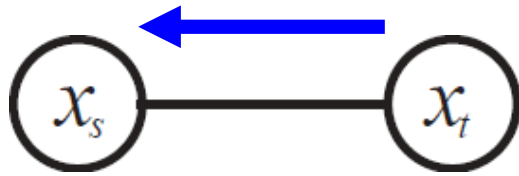
Message



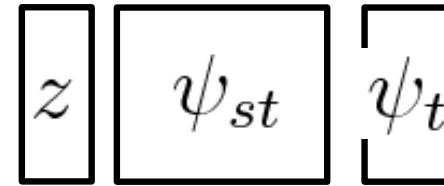
Regular grid of 50 states gives discretization:

$$\mathbb{X} = \{x^{(1)}, \dots, x^{(50)}\}$$

# Particle Selection

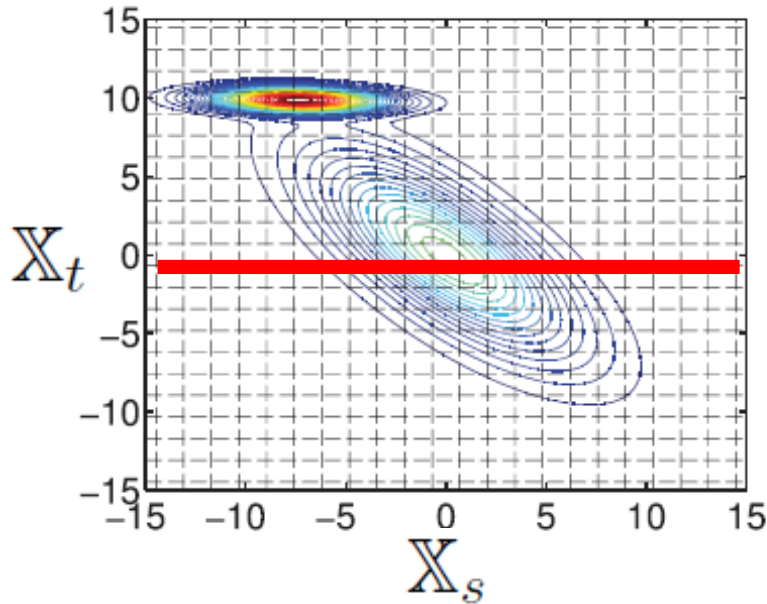


$$\hat{m}_{ts}(z) = \max_{x_t}$$

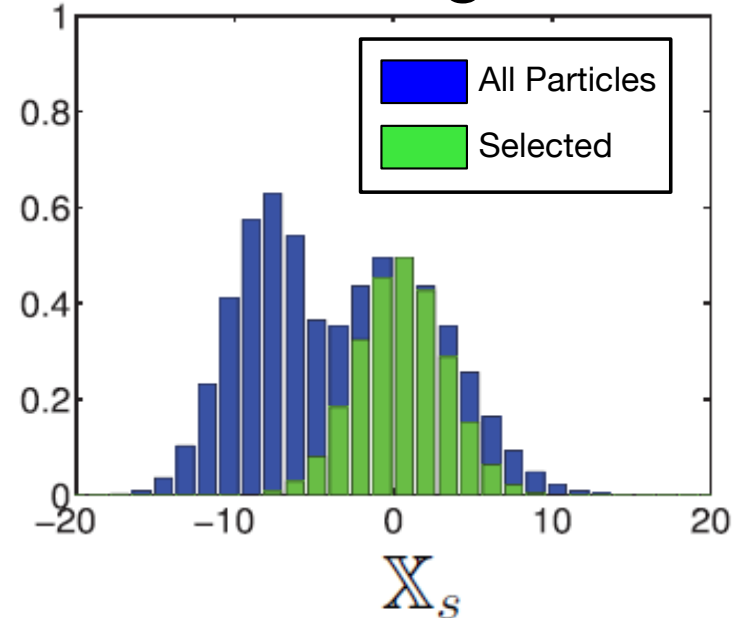


Selection vector

Joint Distribution



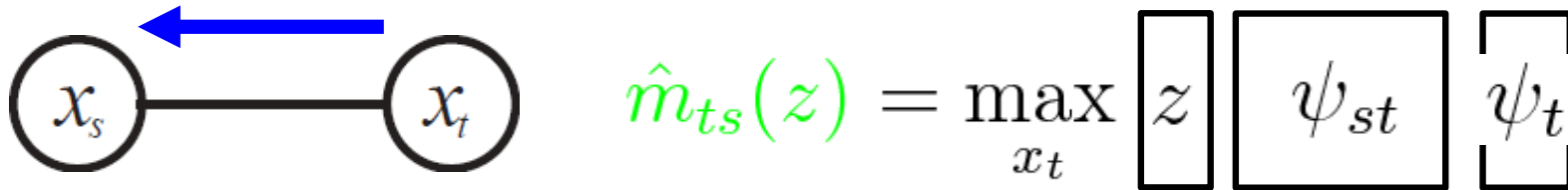
Message



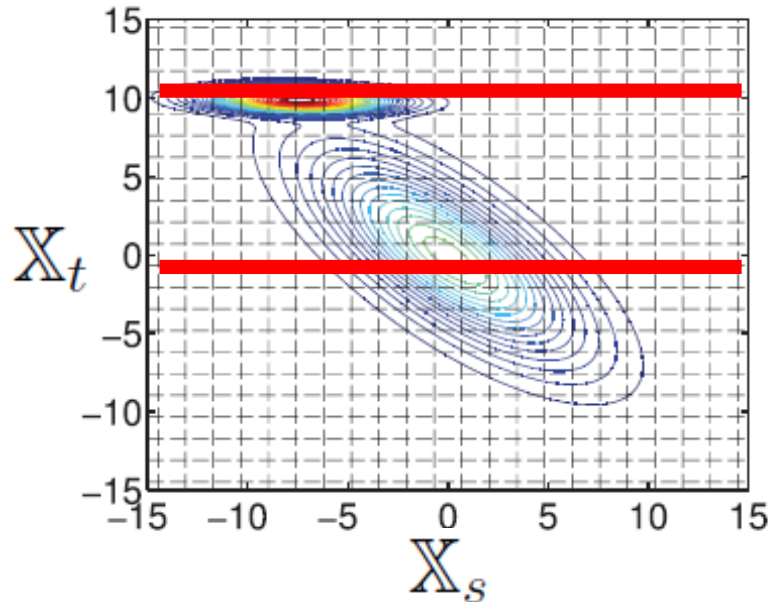
- Indicator vector controls state selection:  $z \in \{0, 1\}^{50}$
- $z(i) = 1$  indicates selected states (red line)



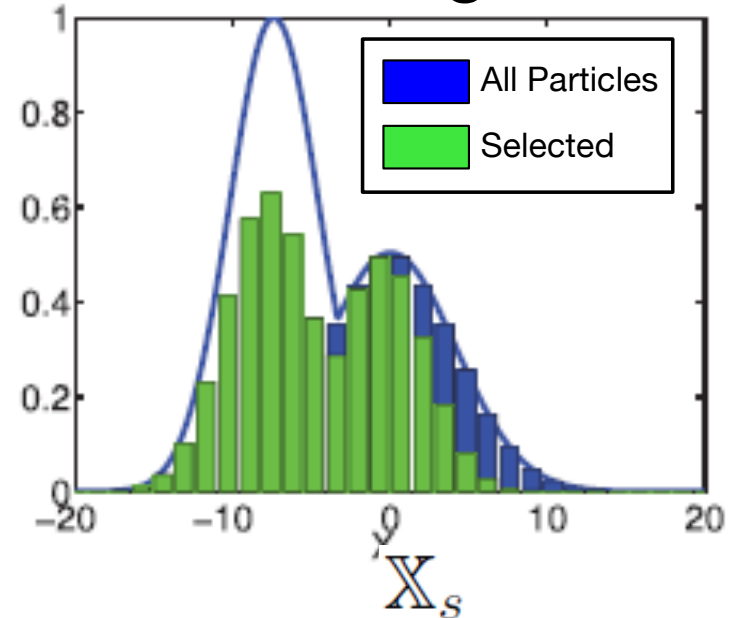
# Particle Selection



Joint Distribution



Message



**Adding states reduces distortion between discrete message vectors.**

# Diverse Particle Selection

Minimize total message distortion:

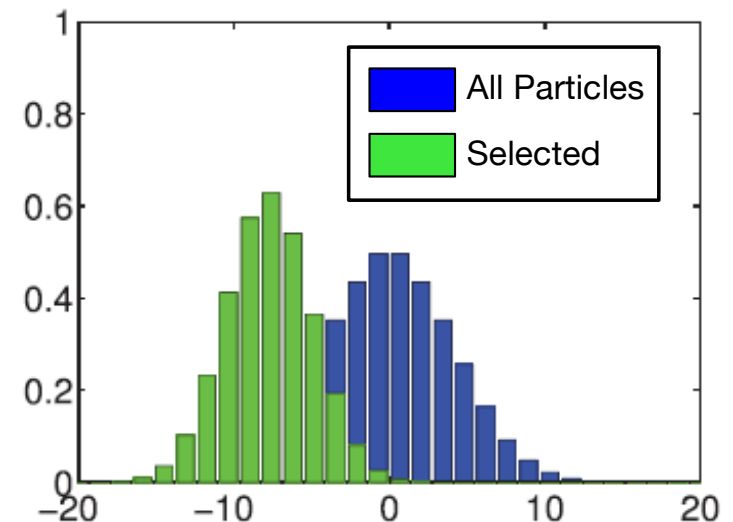
$$\underset{z}{\text{minimize}} \sum_{s \in \Gamma(t)} \sum_{a=1}^{\alpha N} (m_{ts}(a) - \hat{m}_{ts}(a, z))$$

subject to  $\|z\|_1 \leq N, z \in \{0, 1\}^{\alpha N}$

✗ NP-hard

✓ Submodular

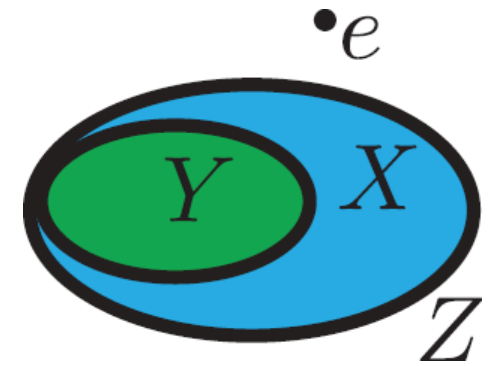
Good approximation qualities.



# Submodularity

Set function  $f : 2^Z \rightarrow \mathbb{R}$  is submodular  
iff **diminishing marginal gains**.

$$f(\underbrace{Y \cup \{e\}}_{\text{Margin}}) - f(Y) \geq f(X \cup \{e\}) - f(X)$$

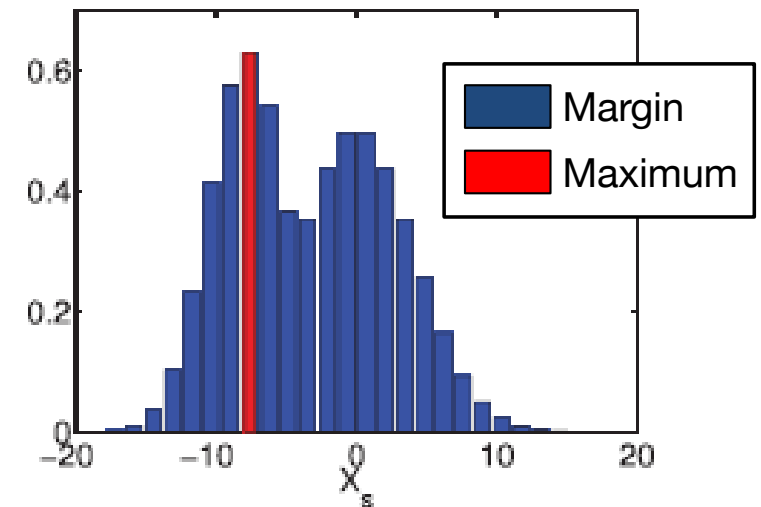
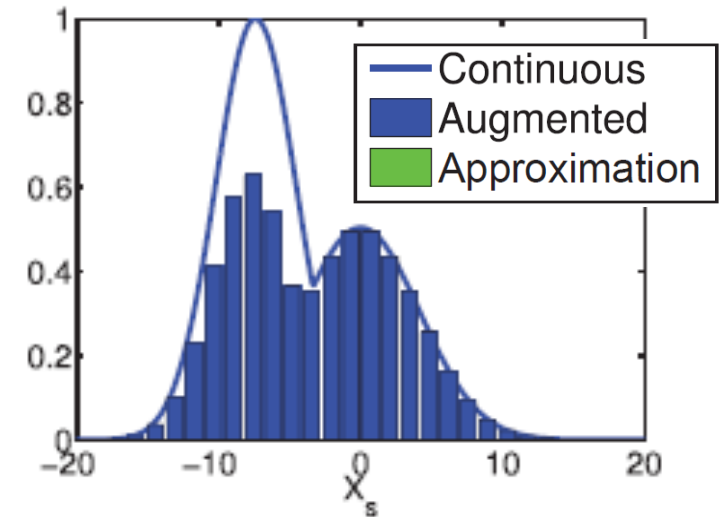
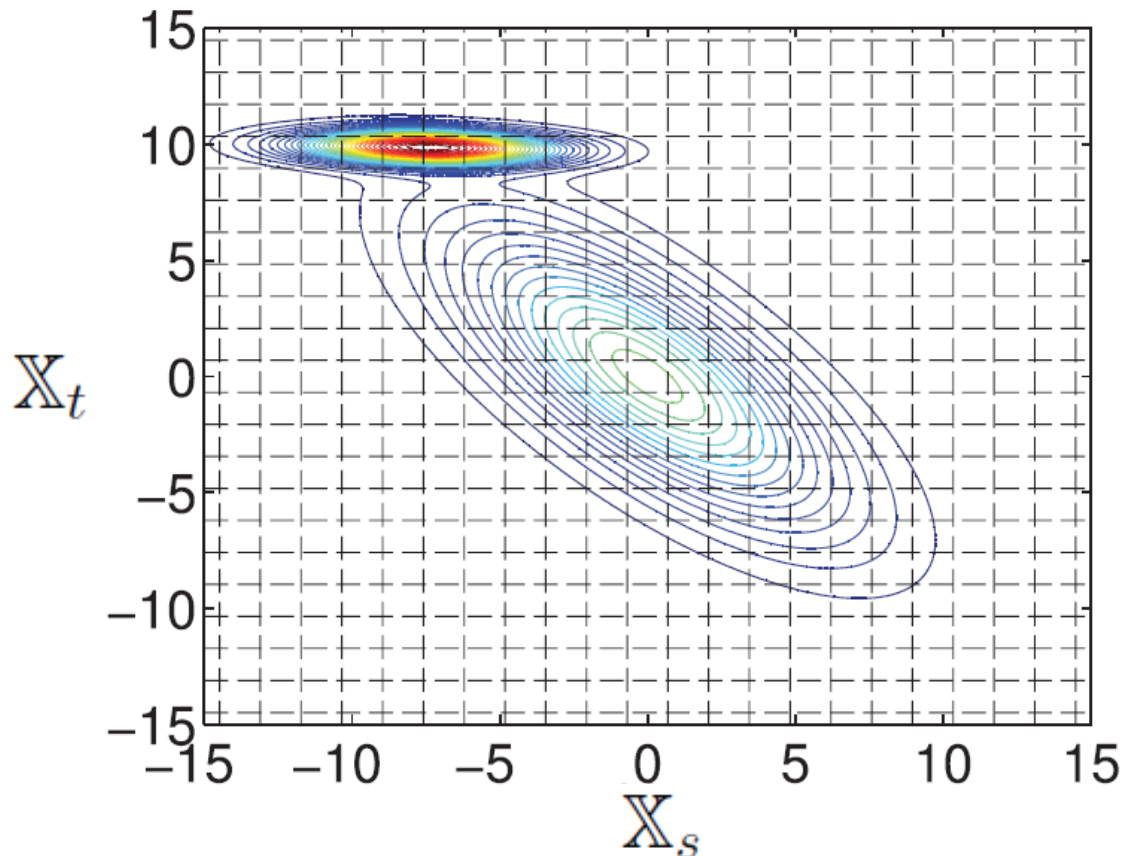


**Diverse particle selection IP equivalent  
to **submodular** maximization.**

- Efficient greedy approximation
- Within  $(1 - 1/e) \approx 63\%$  of optimal

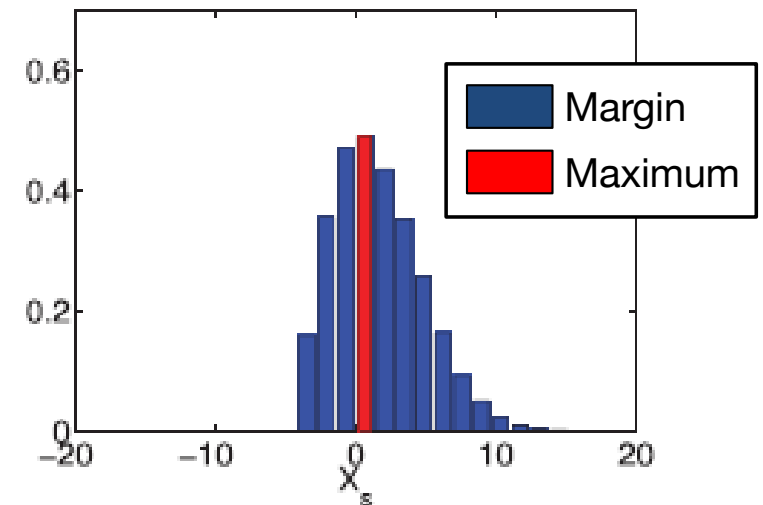
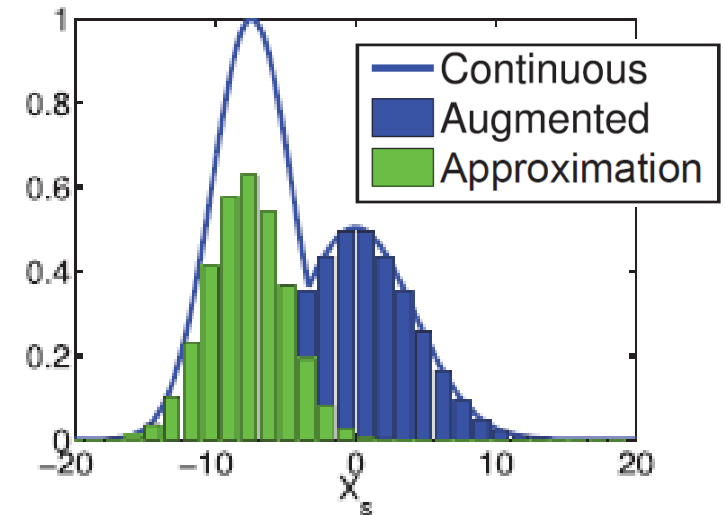
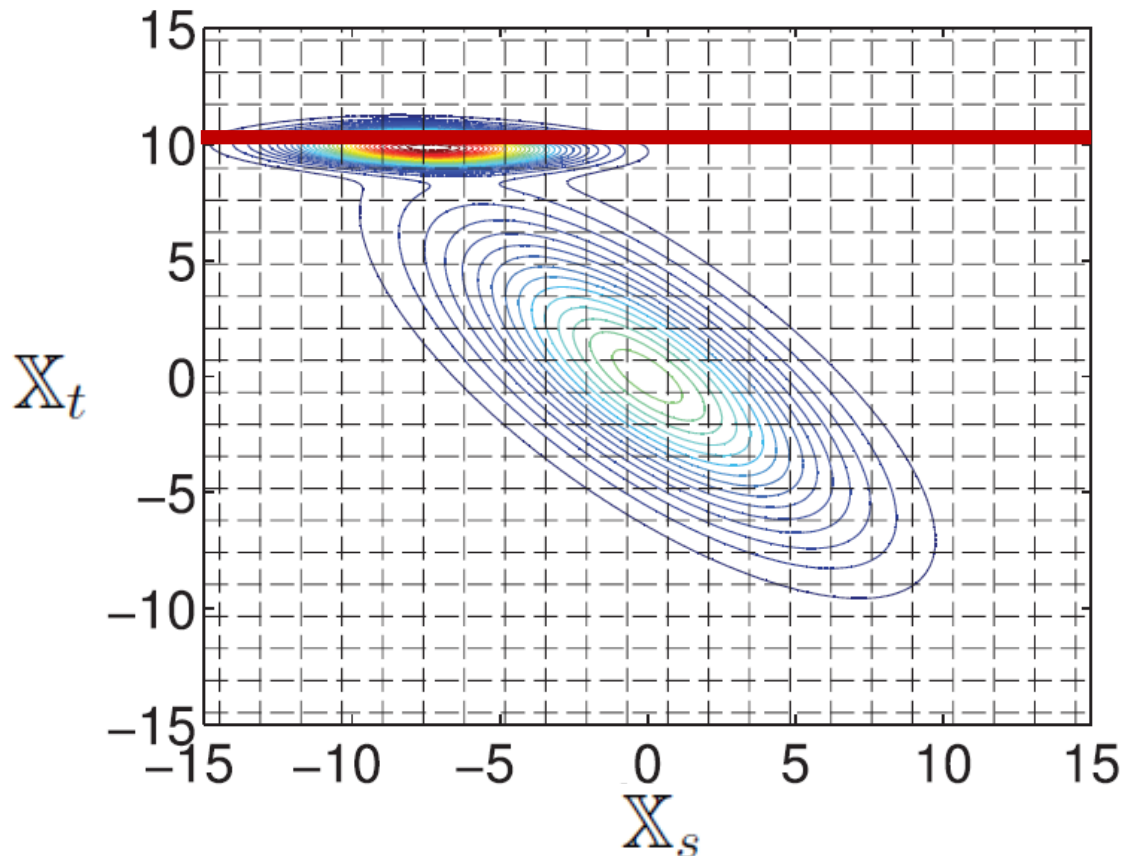
# Greedy Particle Selection

$$\text{minimize}_z \sum_{s \in \Gamma(t)} \sum_{a=1}^{\alpha N} (m_{ts}(a) - \hat{m}_{ts}(a, z))$$



# Greedy Particle Selection

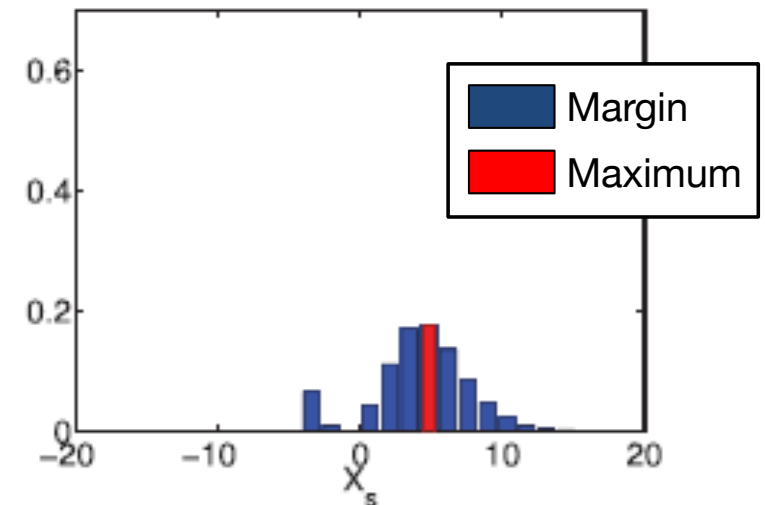
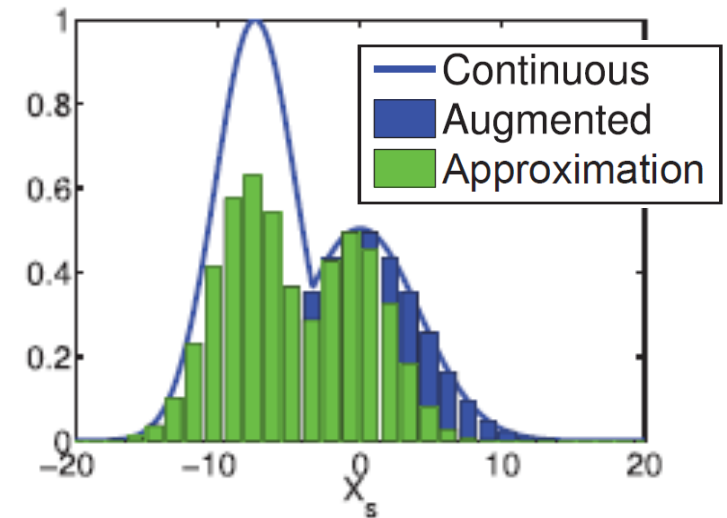
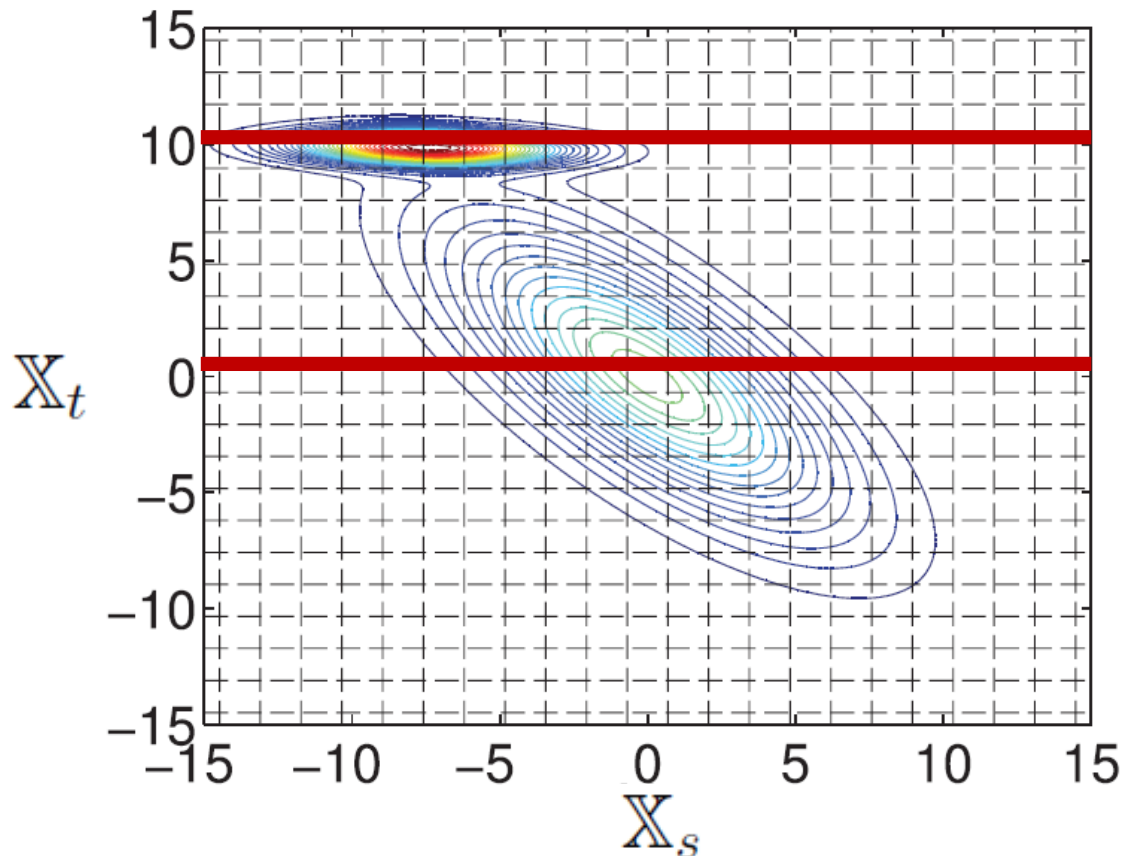
$$\text{minimize}_z \sum_{s \in \Gamma(t)} \sum_{a=1}^{\alpha N} (m_{ts}(a) - \hat{m}_{ts}(a, z))$$





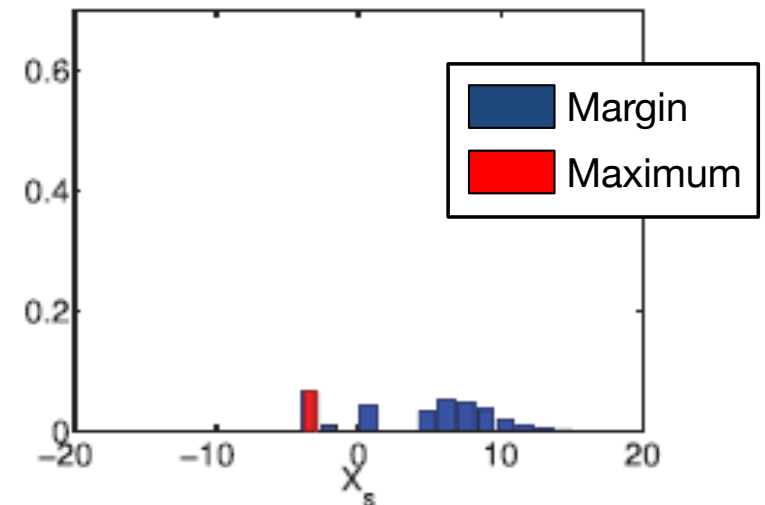
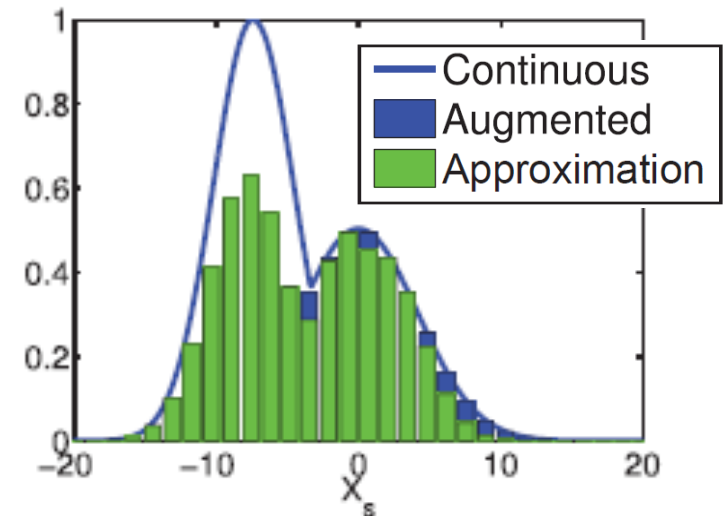
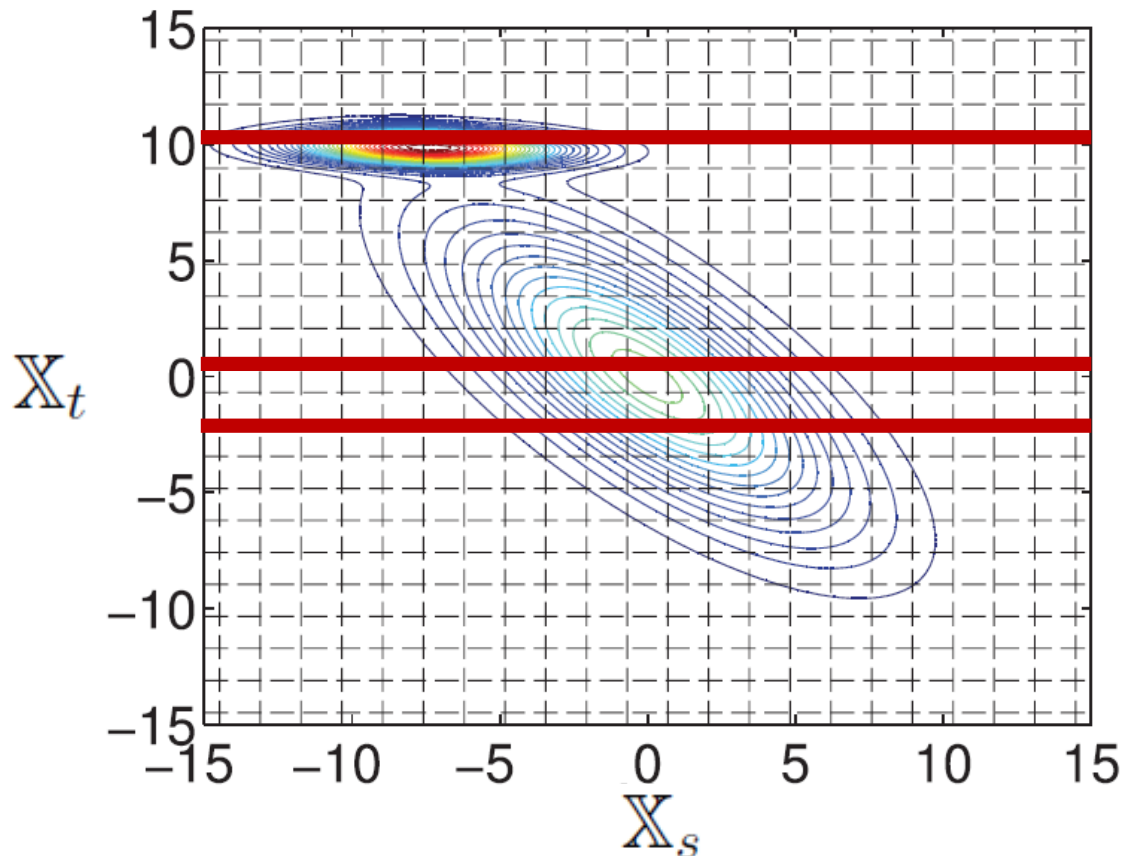
# Greedy Particle Selection

$$\text{minimize}_z \sum_{s \in \Gamma(t)} \sum_{a=1}^{\alpha N} (m_{ts}(a) - \hat{m}_{ts}(a, z))$$



# Greedy Particle Selection

$$\text{minimize}_z \sum_{s \in \Gamma(t)} \sum_{a=1}^{\alpha N} (m_{ts}(a) - \hat{m}_{ts}(a, z))$$

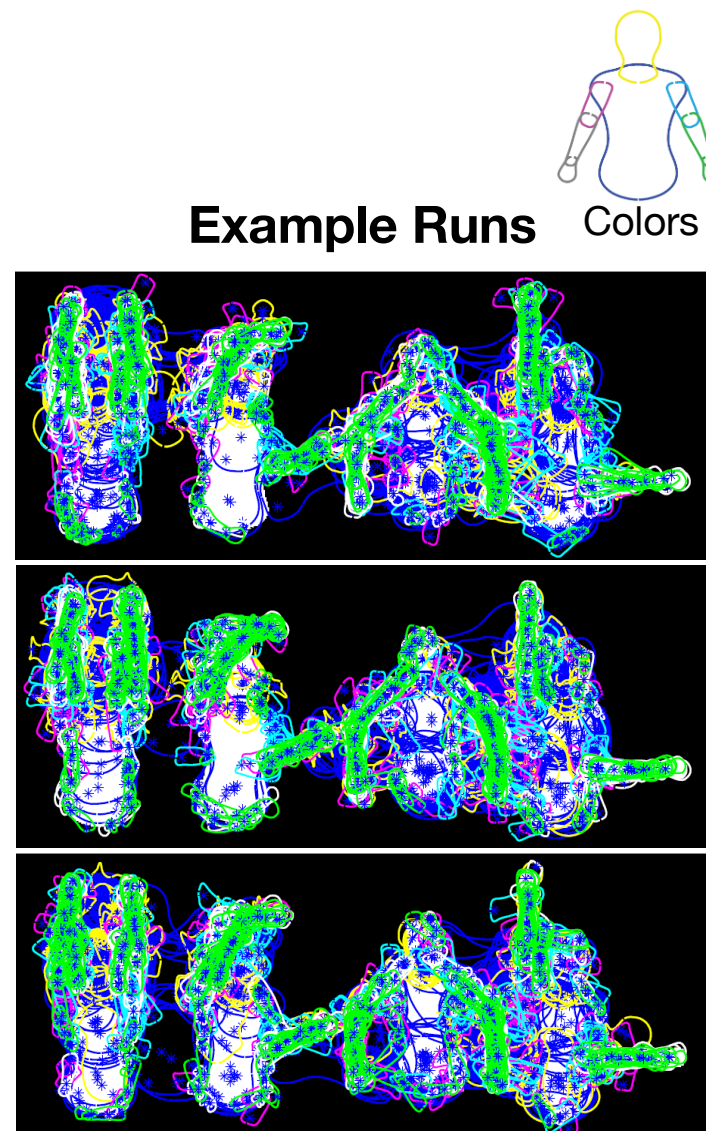


# Diverse Particle Max-Product (D-PMP)



- No explicit diversity constraint
- Objective encourages diversity
- Efficient “*lazy*” greedy algorithm
- Bounds on optimality

Avoids particle degeneracies by maintaining *ensemble of diverse solutions* near local modes.



# Discovering Multiple Hypotheses

*Prior Work Specialized to Discrete Graphical Models*

## **M-Best MAP** *[Nilsson 1998; Yanover and Weiss 2003]*

- Produce  $M$  solutions with highest joint probability
- Typically, these are minor variations of a single mode

## **Diverse M-Best MAP** *[Batra et al. 2012]*

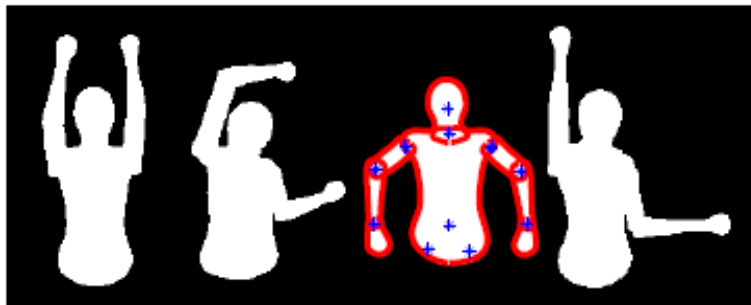
- Externally specified metric used to find probable hypotheses separated by some distance threshold
- Specialized to discrete models, and requires tuning of metrics/thresholds for each graphical model

## **Diverse Particle Max-Product**

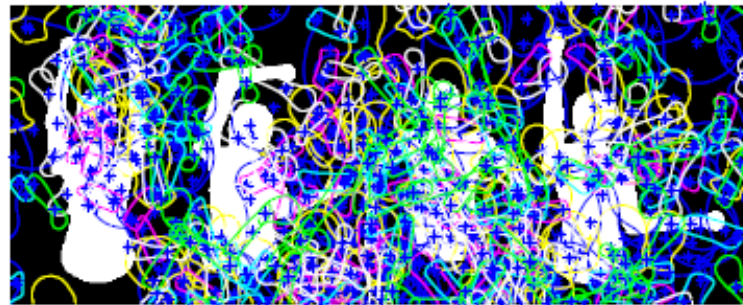
- Tractable for high-dimensional state spaces
- Notion of “distance” arises automatically from model

# Synthetic Images: ICML Puppets

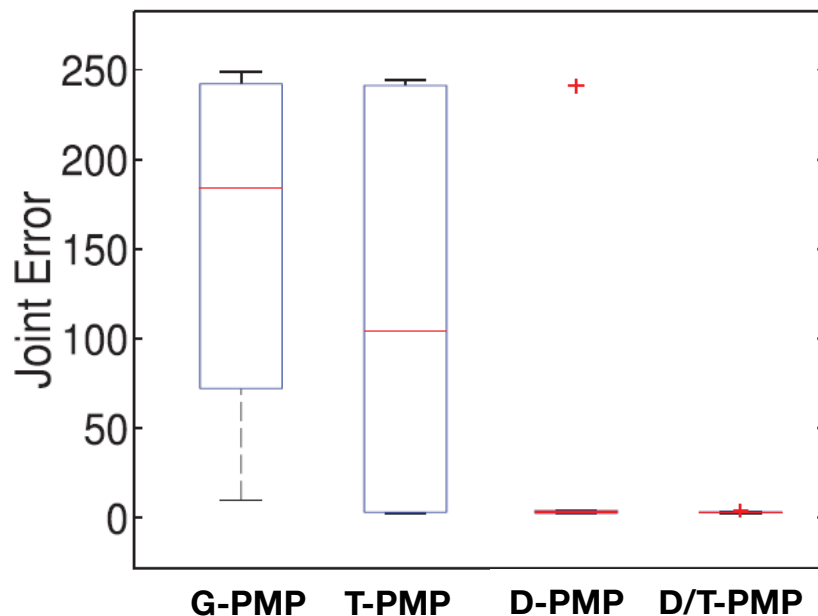
True MAP



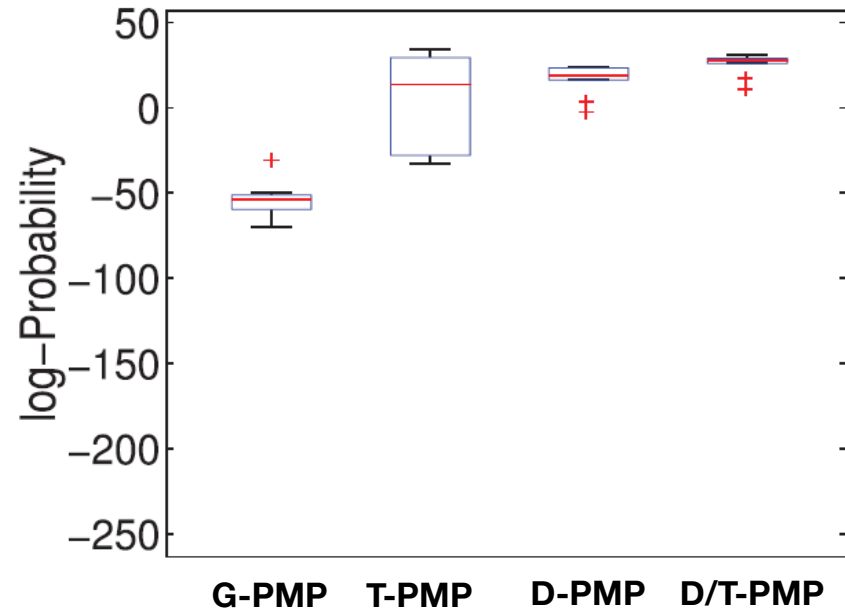
Random Initialization



Pose Error of MAP Estimate



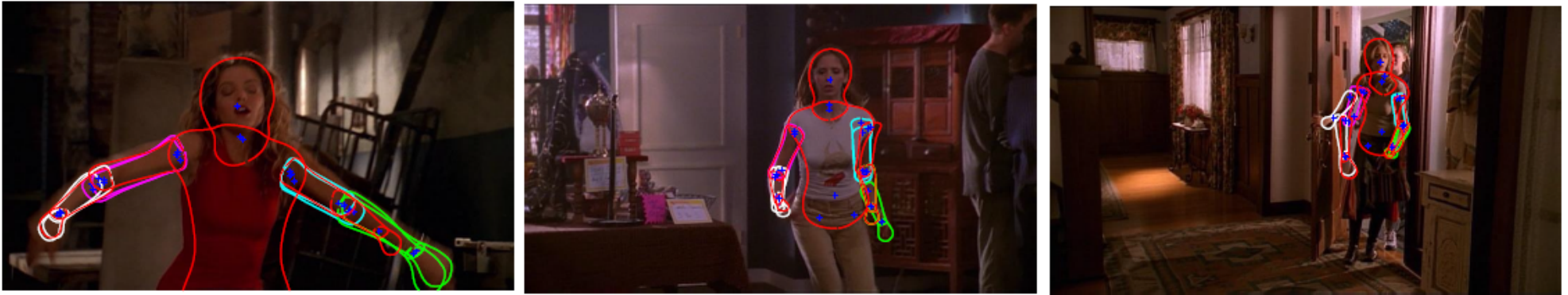
Log Probability of MAP Estimate



*Box plots summarize results from 10 random initializations.*

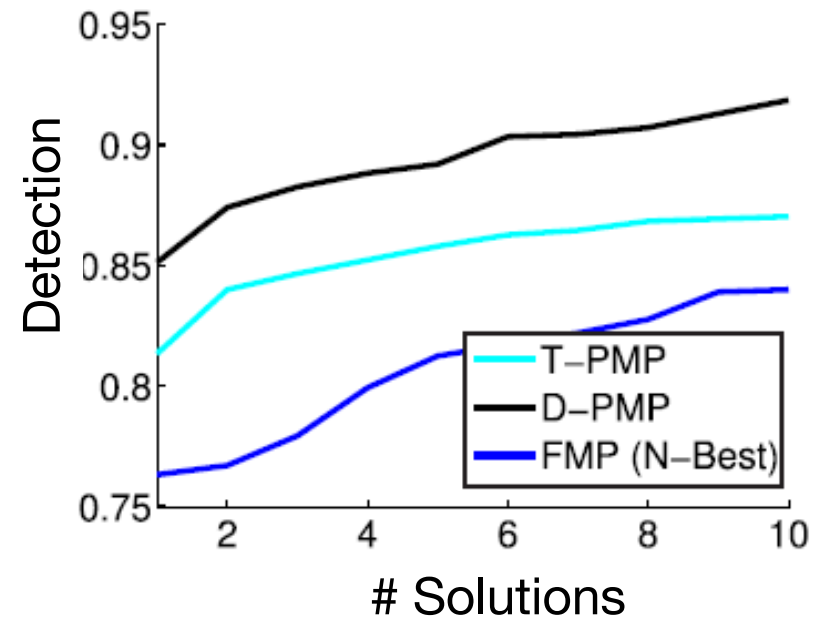


# Real Images (Single Person)

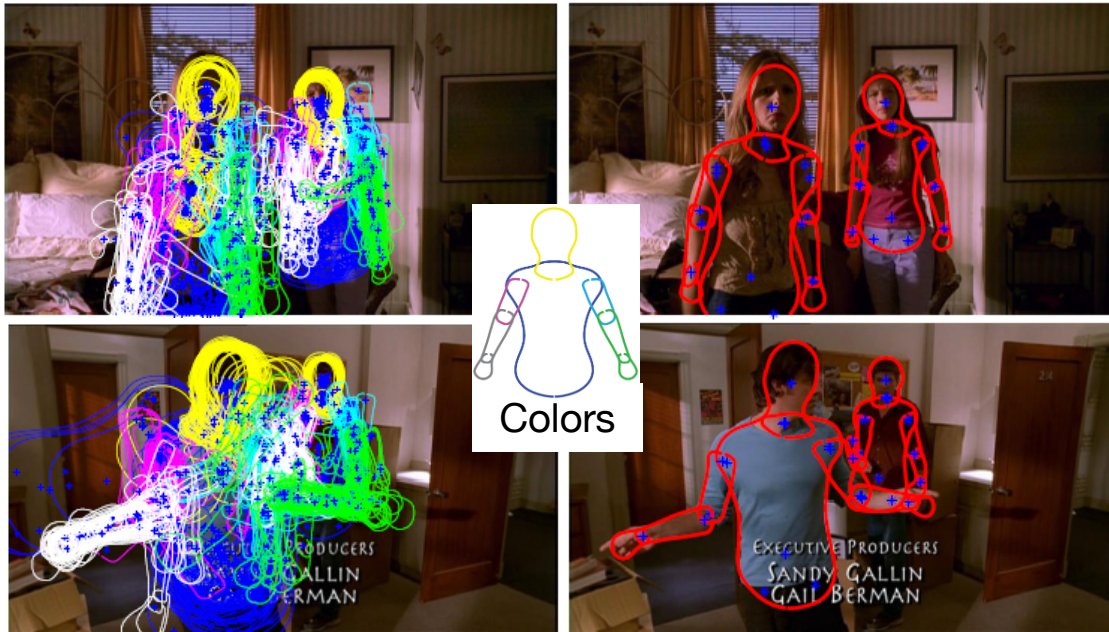


**Top 3 arm hypotheses** MAP estimate, 2<sup>nd</sup> and 3<sup>rd</sup> modes for upper arm (magenta, cyan), lower arm (green, white).

- “Buffy” dataset [Ferrari et al. 2008].
- Detections versus number of ranked hypotheses.
- Baseline: Flexible Mixture of Parts (FMP) [Yang & Ramanan 2013; Park & Ramanan 2011]

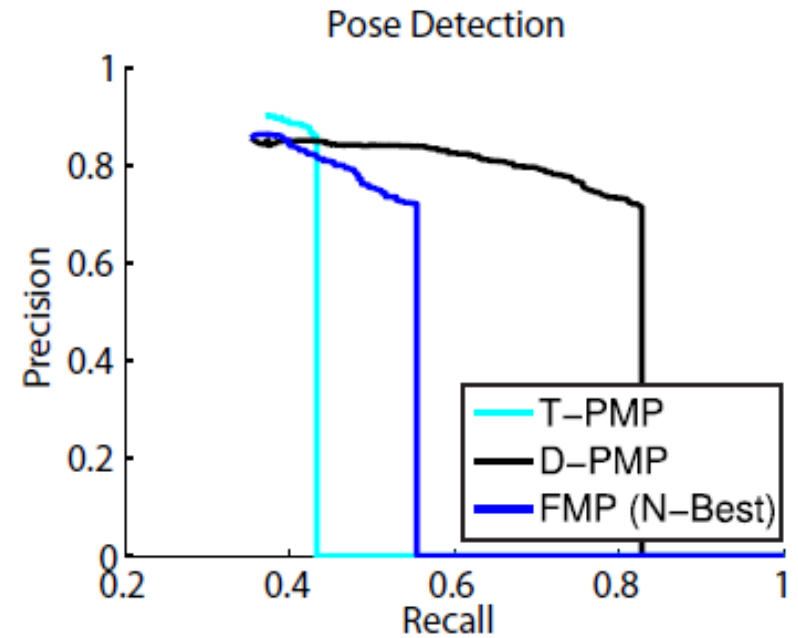


# Real Images (Multiple People)



D-PMP Particles

Mode Estimates



Precision-Recall for multi-person frames:

**T-PMP** : High precision, low recall, particles on one figure

**D-PMP** : Outperforms **FMP** and other particle methods

Note: G-PMP not reported due to poor performance.

# D-PMP for 3D Mesh Alignment

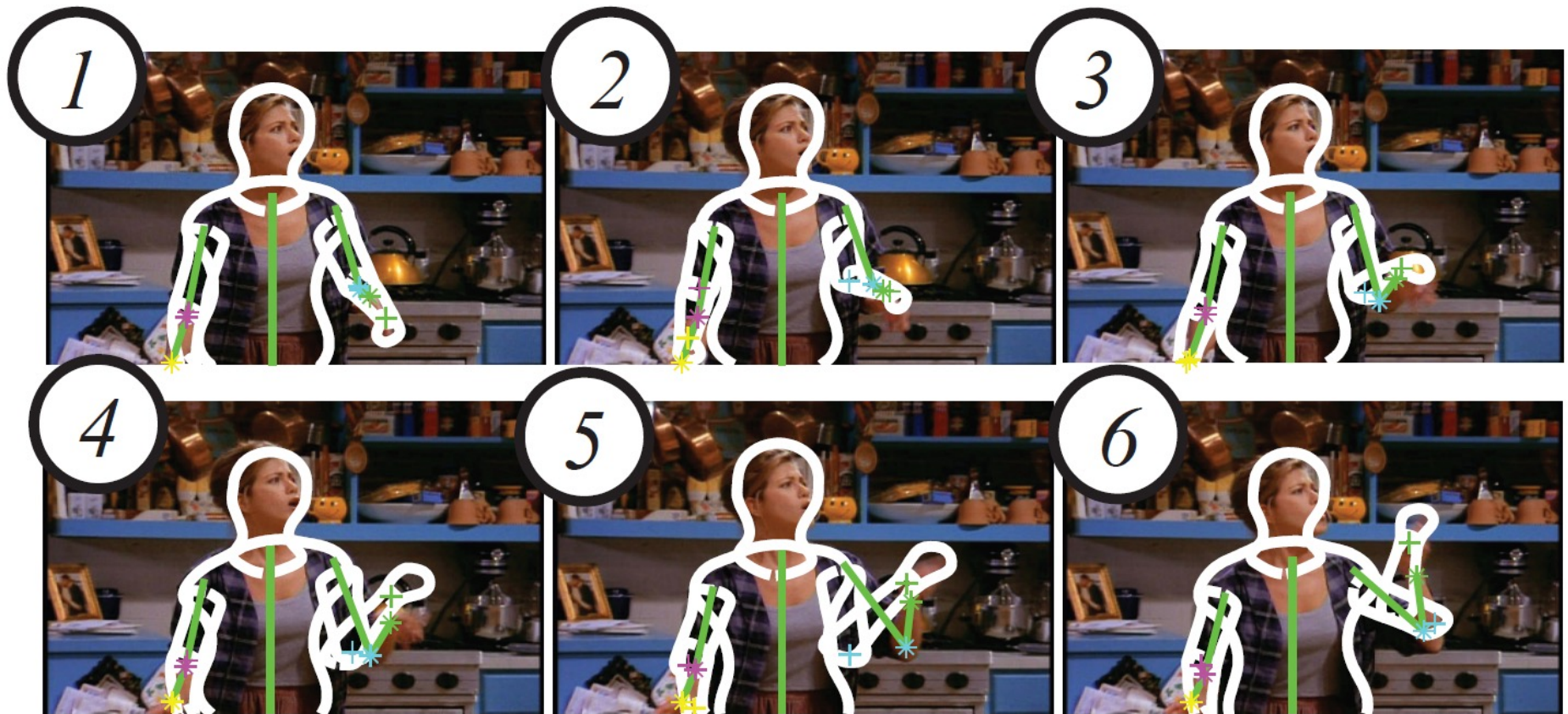


*Independent work by Zuffi & Black, appeared at CVPR 2015.*



# Articulated Pose Tracking

**Prior work fails to show improvement by incorporating motion model.**



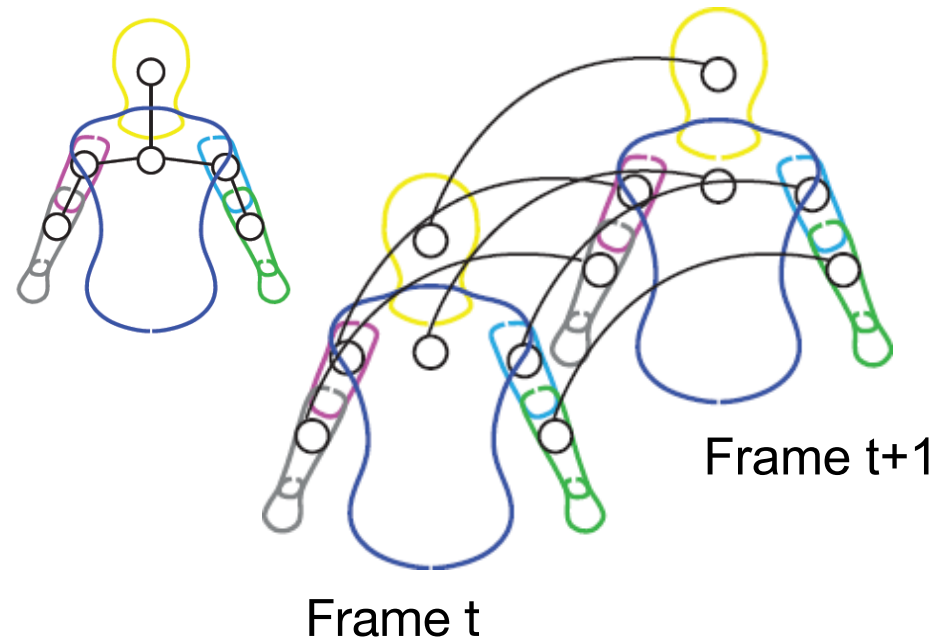
**This is a failure of inference...**

# Articulated Pose Tracking

## Data and Optical Flow

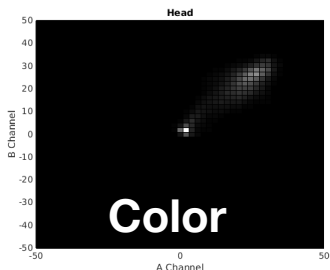
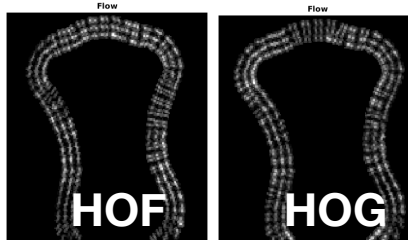


Extension of the *Flowing Puppets* model [Zuffi et al., 2013]



## Part Likelihood

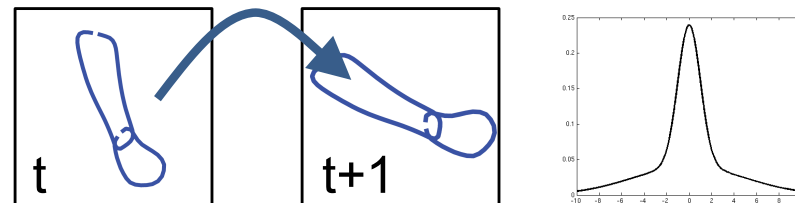
**Gradients:** Encode object and motion boundaries via HOG / HOF.



**Appearance:** 2D histogram of A/B color channels in  $L^*a^*b^*$  space. Luminance ignored.

## Prior

**Part Motion:** Scale mixture captures heavy tailed statistics of motion between frames.

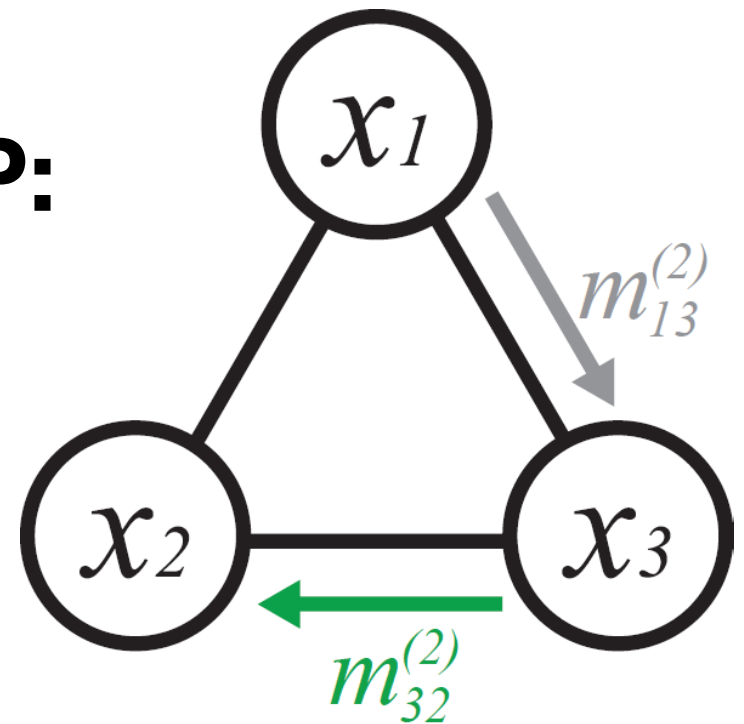


**Structural prior identical to DS.**

# Loopy Max-Product BP

Many interesting models exhibit *cyclic* dependency structure...

**Loopy Max-Product BP:**  
Iteratively update  
until converged.

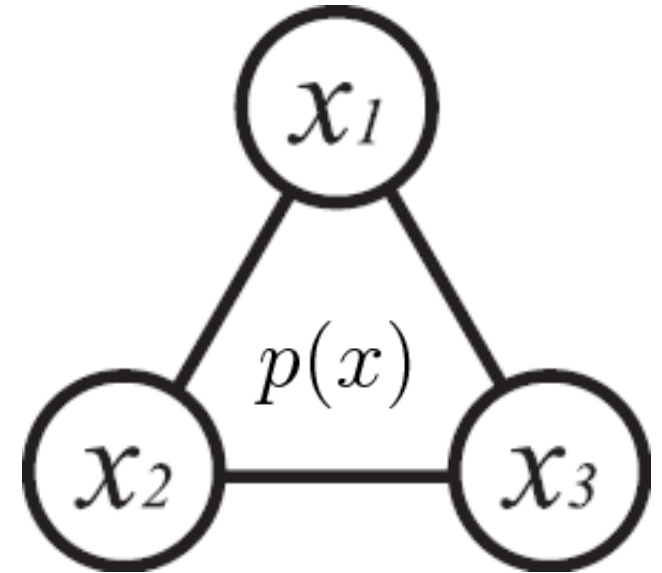
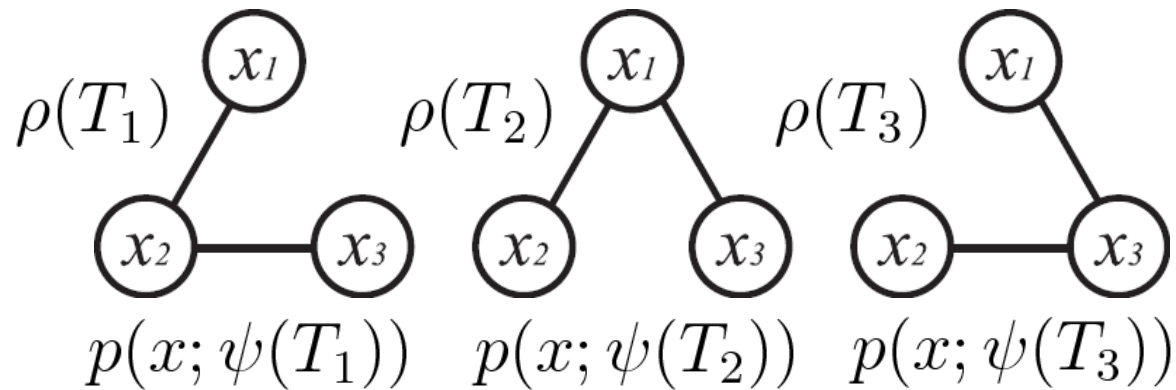


State-of-the-art decoding for error correcting codes  
but **may perform poorly in general.**



# MAP Probability Bound

## Spanning Tree Distribution



Bound MAP via Jensen's Inequality:

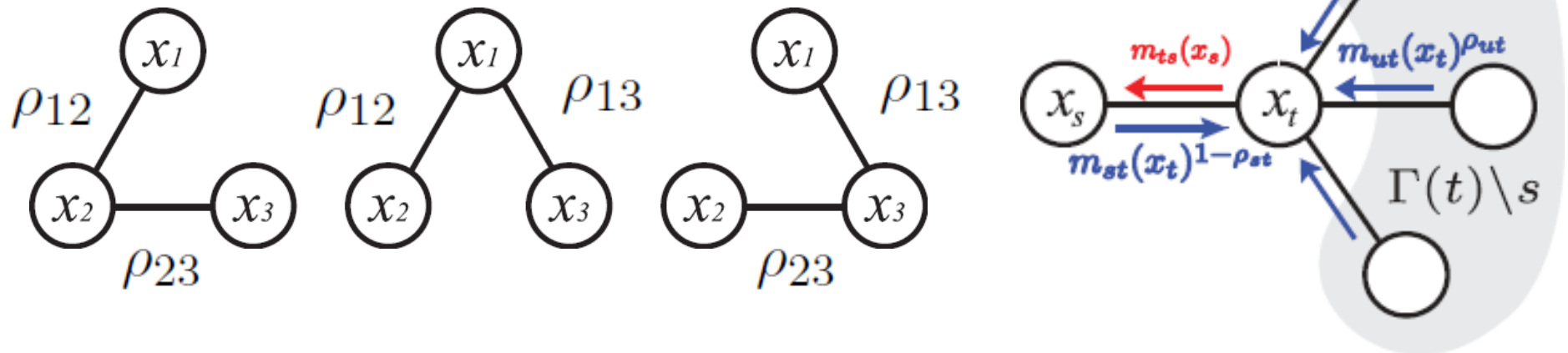
$$\max_x \log p(x) \leq \sum_T \rho(T) \max_x \log p(x; \psi(T))$$

Dual Problem:

$$\text{minimize}_{\psi} \sum_T \rho(T) \max_x \log p(x; \psi(T))$$

# Reweighted Max-Product (RMP)

## Edge Appearance



$$m_{ts}(x_s) = \max_{x_t} \psi_t(x_t) \psi_{st}(x_s, x_t) \frac{1}{\rho_{st}} \frac{\prod_{u \in \Gamma(t) \setminus s} m_{ut}(x_t)^{\rho_{ut}}}{m_{st}(x_t)^{1-\rho_{st}}}$$

Solve dual problem via *reweighted*  
message passing

# RMP Bound Tightness

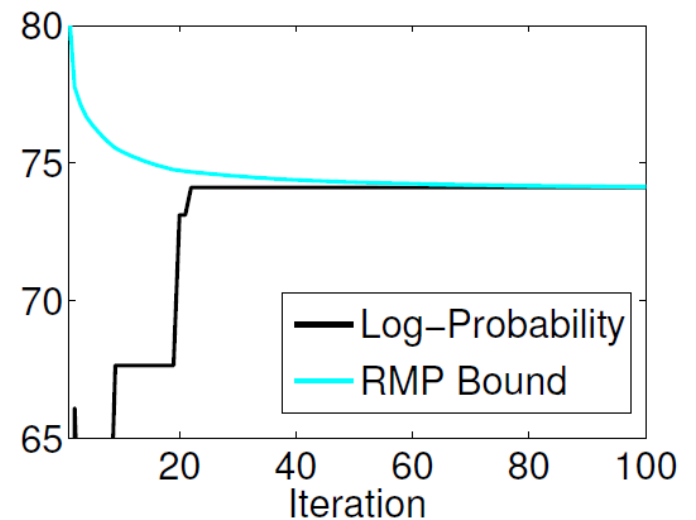
Pseudo-Max-Marginal distribution:

$$\nu_s(x_s) \propto \psi_s(x_s) \prod_{u \in \Gamma(s)} m_{us}(x_s)^{\rho_{us}} \approx q_s(x_s)$$

Consistent maximizer:

$$x_s^* = \operatorname{argmax}_{x_s} \nu_s(x_s)$$

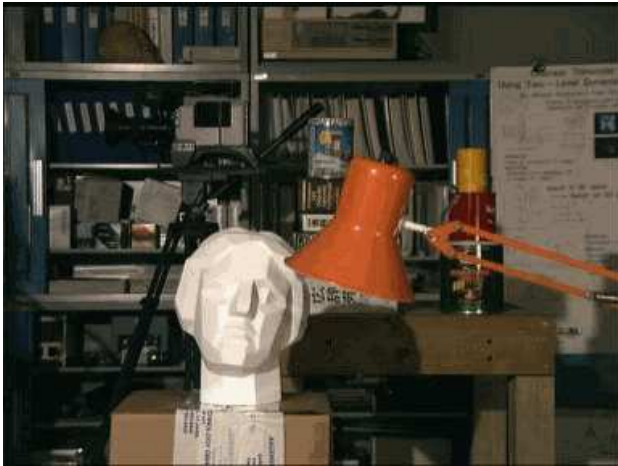
$$(x_s^*, x_t^*) = \operatorname{argmax}_{x_s, x_t} \nu_{st}(x_s, x_t)$$



RMP bound tight and  $x^*$  global MAP:

$$\max_x \log p(x) = \sum_T \rho(T) \max_x \log p(x; \psi(T))$$

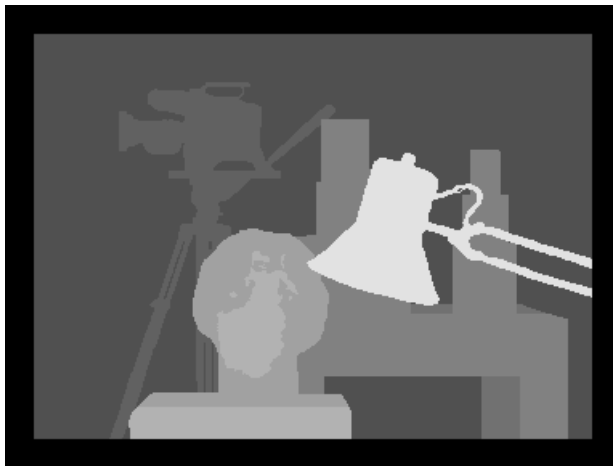
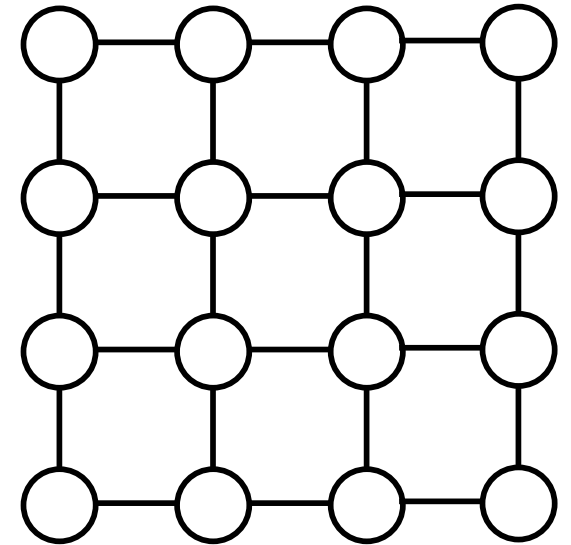
# Reweighted BP & Stereo Vision



Left

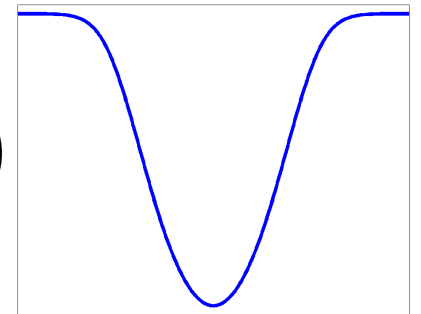


Right



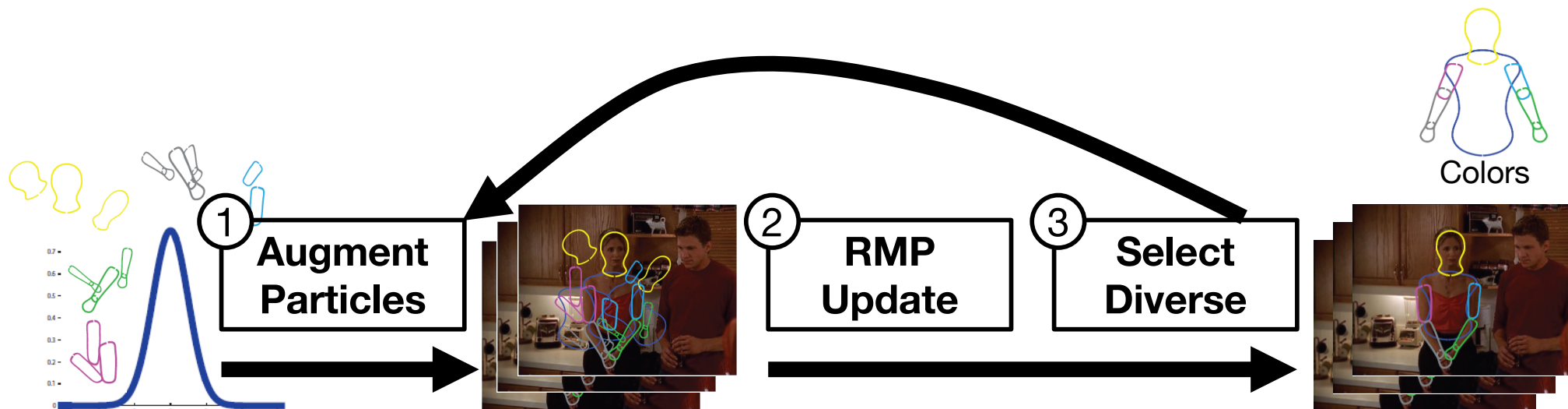
Disparity

$$-\log \psi_{st}(x_s, x_t)$$

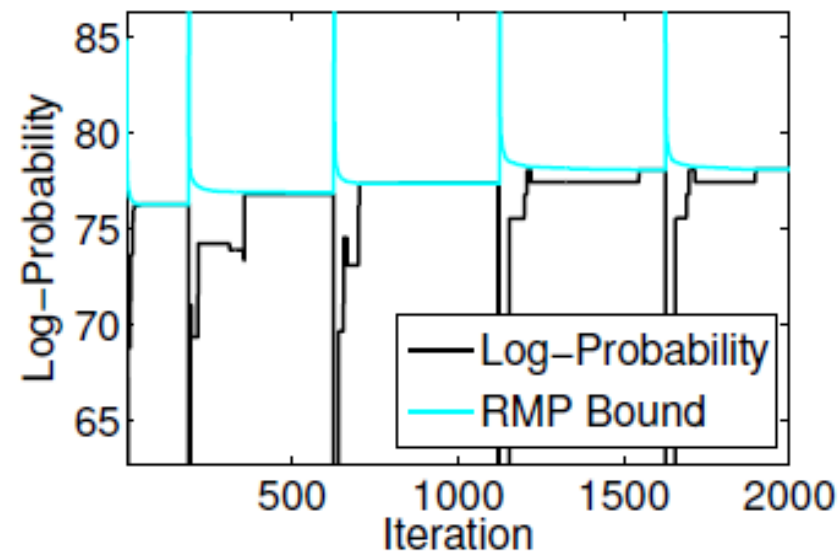


- State space is horizontal displacement (disparity) between corresponding pixels in aligned images (~50 options)
- Yanover, Meltzer, Weiss (JMLR 2006) show reweighted max-product finds global MAP in ~90% of test instances

# Loopy Particle Max-Product



Select diverse subset  
and repeat...



# Diverse Particle Selection

Minimize reweighted message distortion:

$$\underset{z}{\text{minimize}} \sum_{s \in \Gamma(t)} \sum_{a=1}^{\alpha N} (m_{ts}(a)^{\rho_{st}} - \hat{m}_{ts}(a, z)^{\rho_{st}})$$

$$\text{subject to } \|z\|_1 \leq N, z \in \{0, 1\}^{\alpha N}$$

- Accounts for spanning tree distribution
- Remains submodular
- Same greedy approximation



# Pseudo-Max-Marginal Error

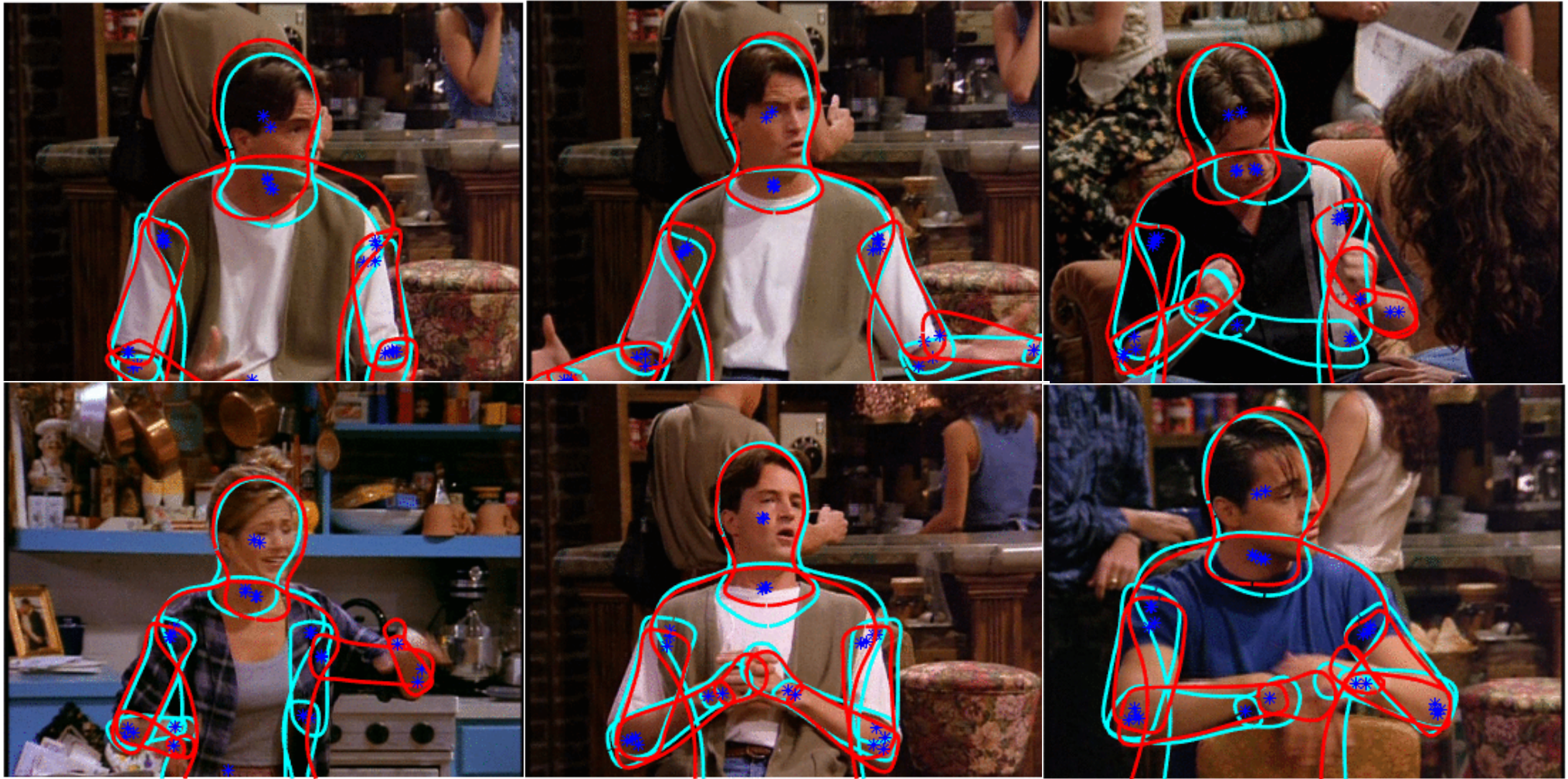
**Selection IP objective upper bounds pseudo-max-marginal distortion.**

$$\|\nu_s - \hat{\nu}_s\|_1 \leq \sum_{t \in \Gamma(s)} \sum_{a=1}^{\alpha N} (m_{ts}(a)^{\rho_{st}} - \hat{m}_{ts}(a)^{\rho_{st}})$$

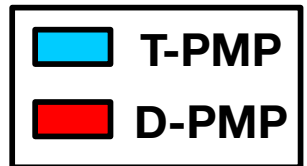
Recall pseudo-max-marginal definitions:

$$\nu_s(a) \propto \psi_s(a) \prod_{t \in \Gamma(s)} m_{ts}(a) \quad \hat{\nu}_s(a) \propto \psi_s(a) \prod_{t \in \Gamma(s)} \hat{m}_{ts}(a)$$

# VideoPose2 Experiments



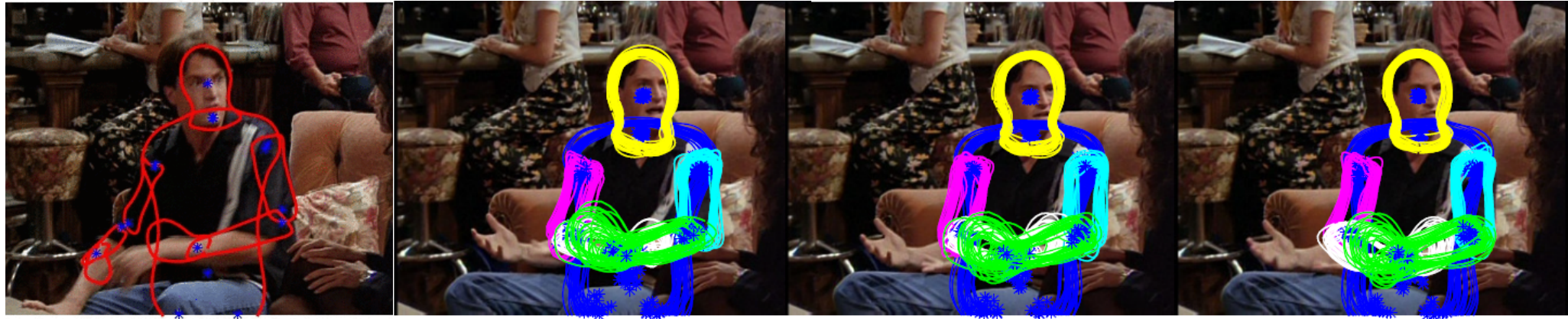
**Comparison on VideoPose2  
dataset of ~2,000 video frames  
from TV shows [Sapp et al., 2011]**





# Pose Tracking Particles

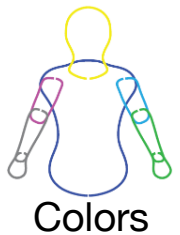
## T-PMP



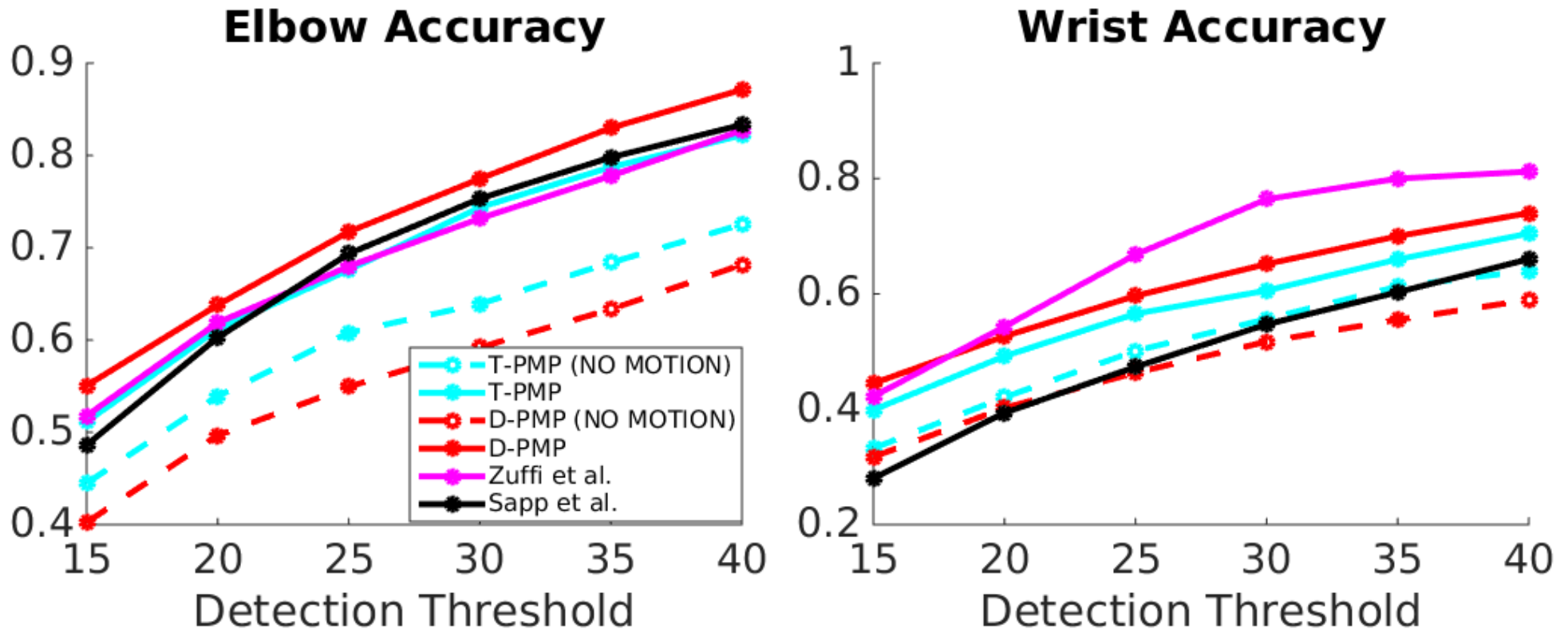
## D-PMP Both right arm hypotheses



Greater diversity in particles allows  
D-PMP to reason more globally

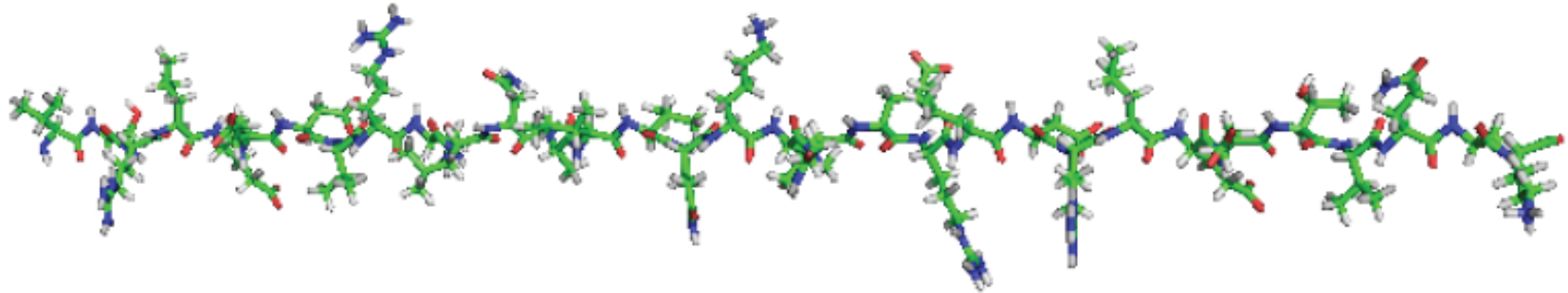


# VideoPose2 Experiments [Sapp et al. 2011]

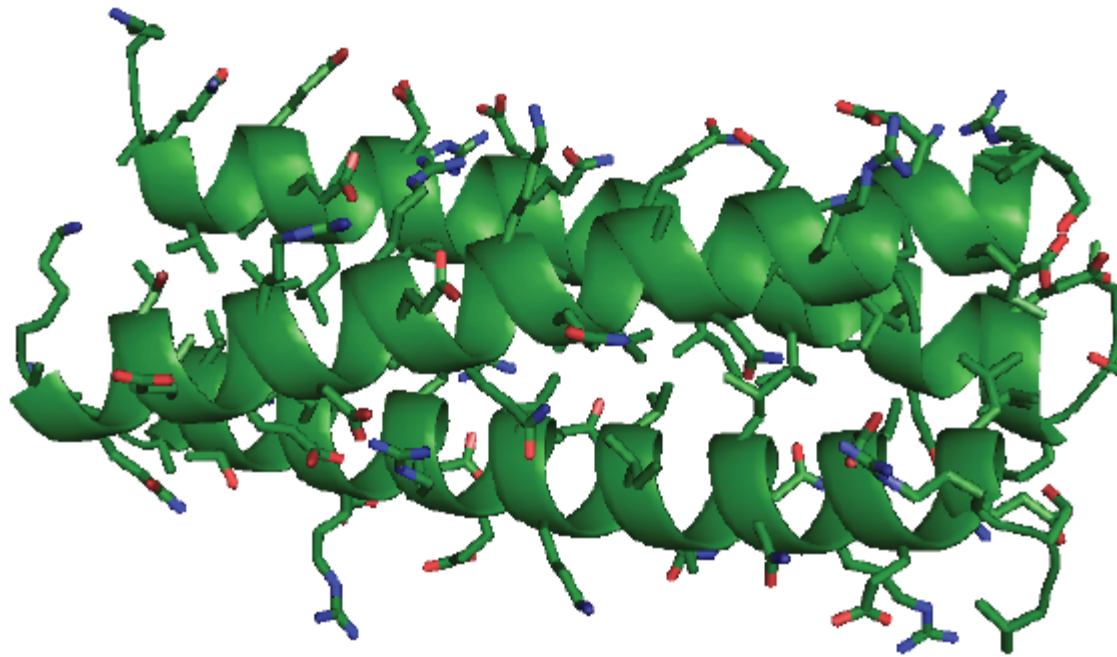


- Superior to static image estimates (---, ---)
- Clear improvement over Sapp et al. baseline
- **D-PMP** superior to **Flowing Puppets** in close detection ranges. Looking at failure cases.

# Protein Structure Prediction



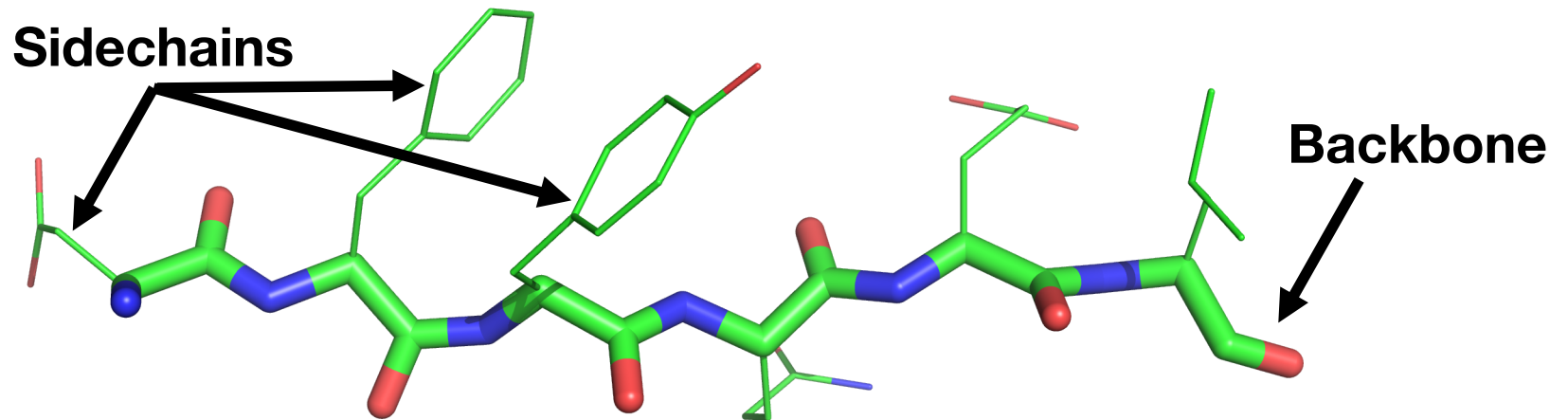
V-S-R-L-E-E-D-V-R-N-L-N-A-I-V-Q-K-L-Q-E-R-L-D-R-L-E-E-T-V-Q-A-K



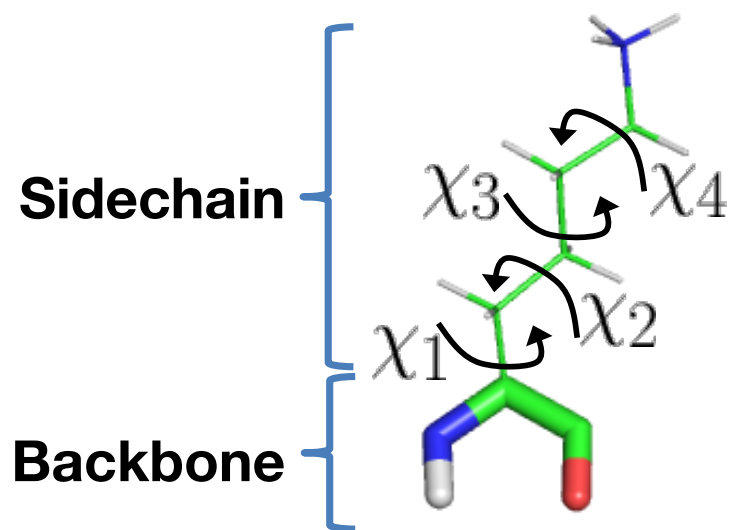
All information for predicting 3D structure encoded in amino acid sequence and physics



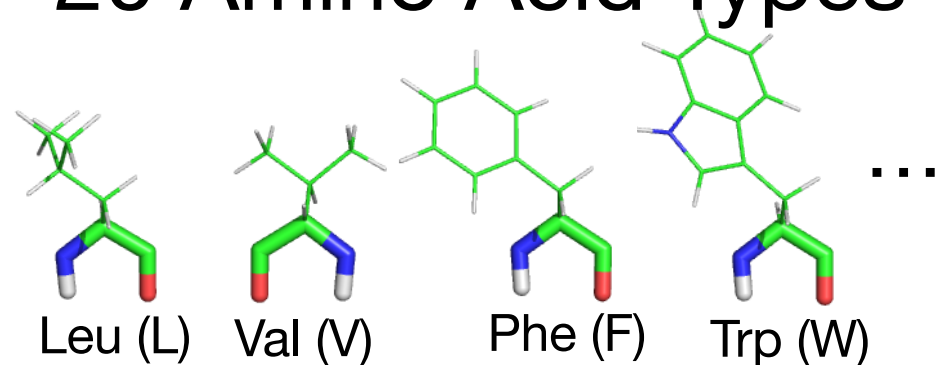
# Protein Side Chains



**Side chain prediction: Estimate side chains given fixed backbone.**

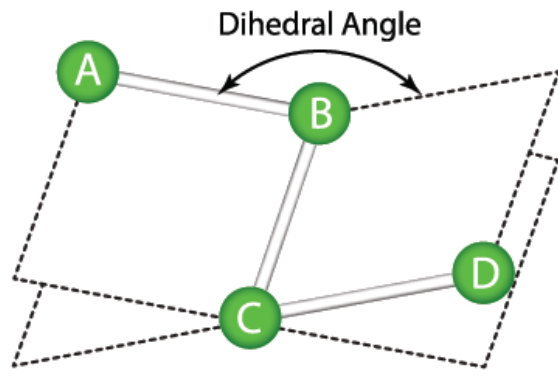


20 Amino Acid Types





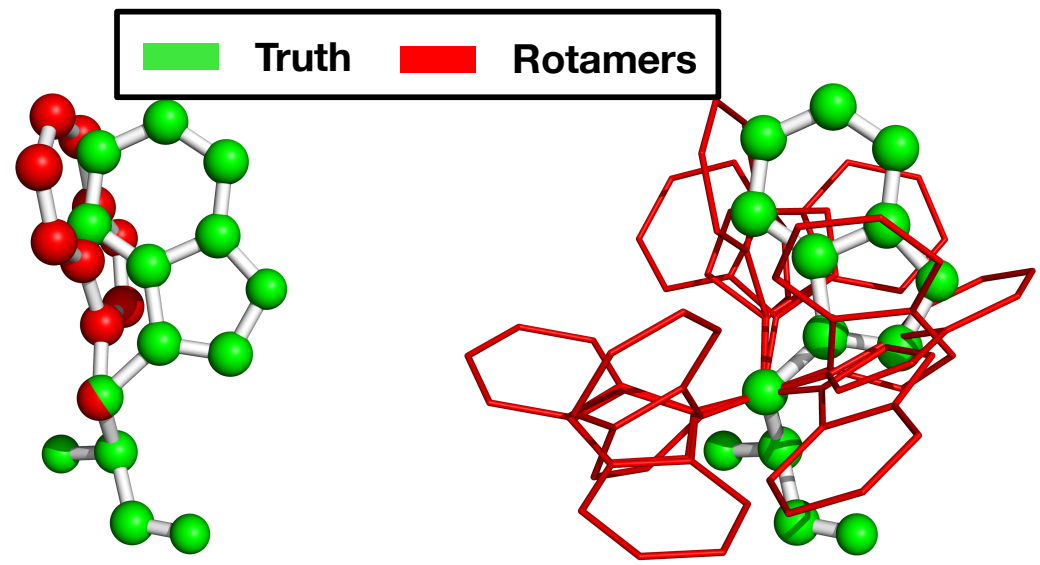
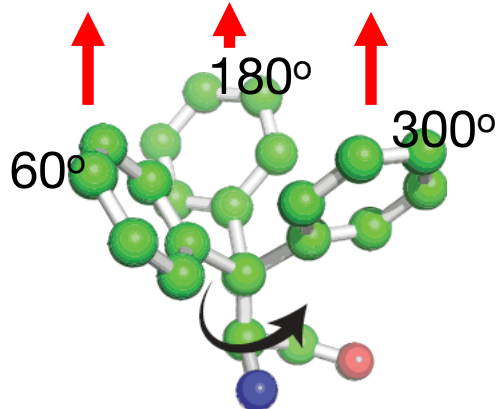
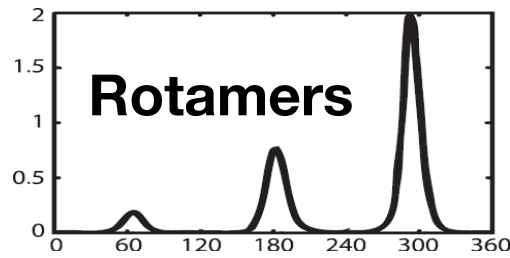
# Dihedrals and Rotamers



## Dihedral Angles:

- Compact angular encoding
- 1D-4D continuous state

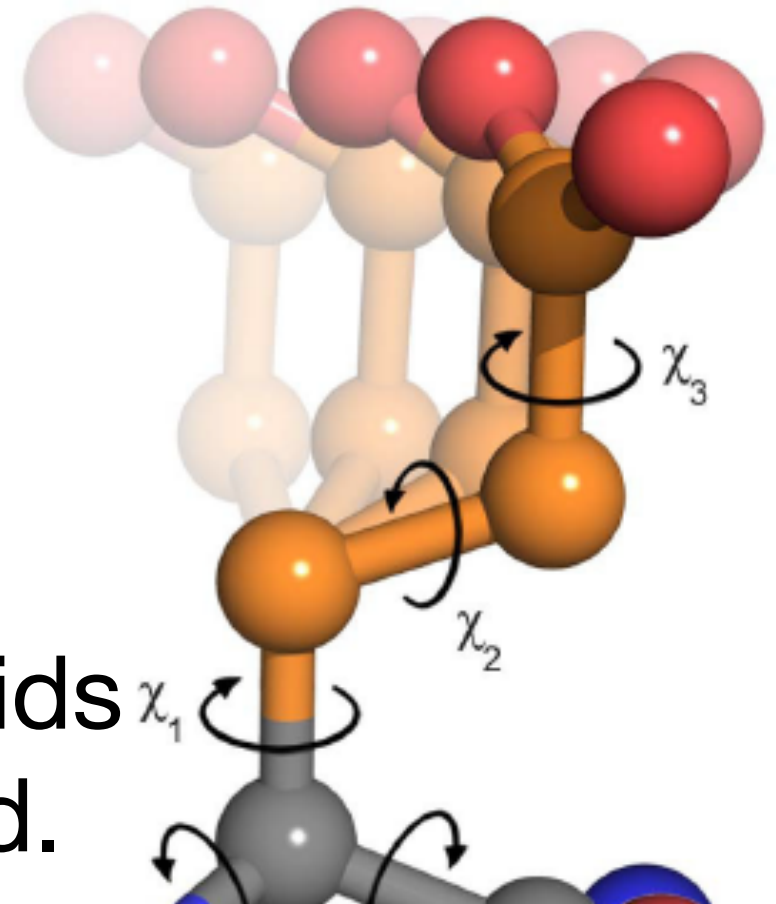
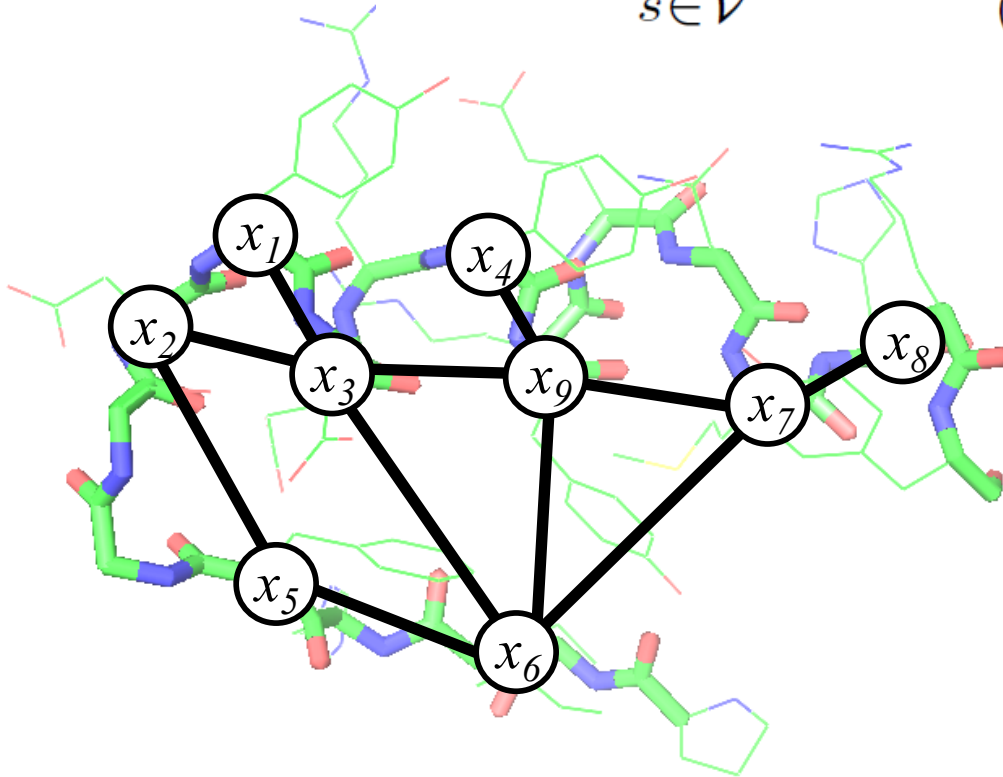
**Rotamer discretization based on marginal statistics fails to capture fine details...**



[Shapovalov & Dunbrack 2007]

# Side Chain Prediction

$$p(x) \propto \prod_{s \in \mathcal{V}} \psi_s(x_s) \prod_{(s,t) \in \mathcal{E}} \psi_{st}(x_s, x_t)$$

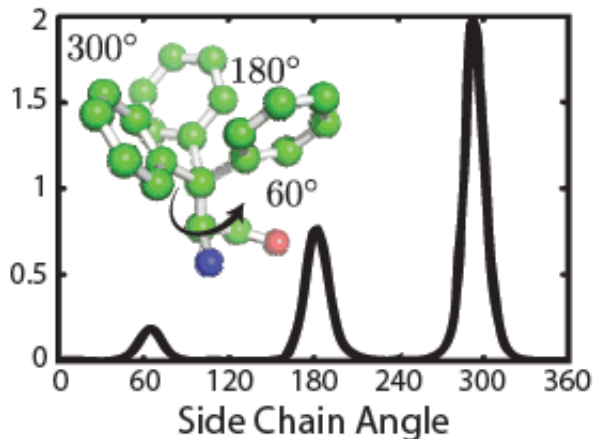


Edges between amino acids within distance threshold.

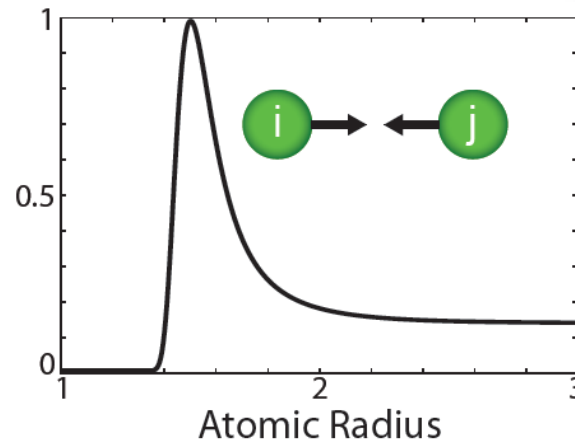
# Side Chain Prediction

$$p(x) \propto \prod_{s \in \mathcal{V}} \psi_s(x_s) \prod_{(s,t) \in \mathcal{E}} \psi_{st}(x_s, x_t)$$

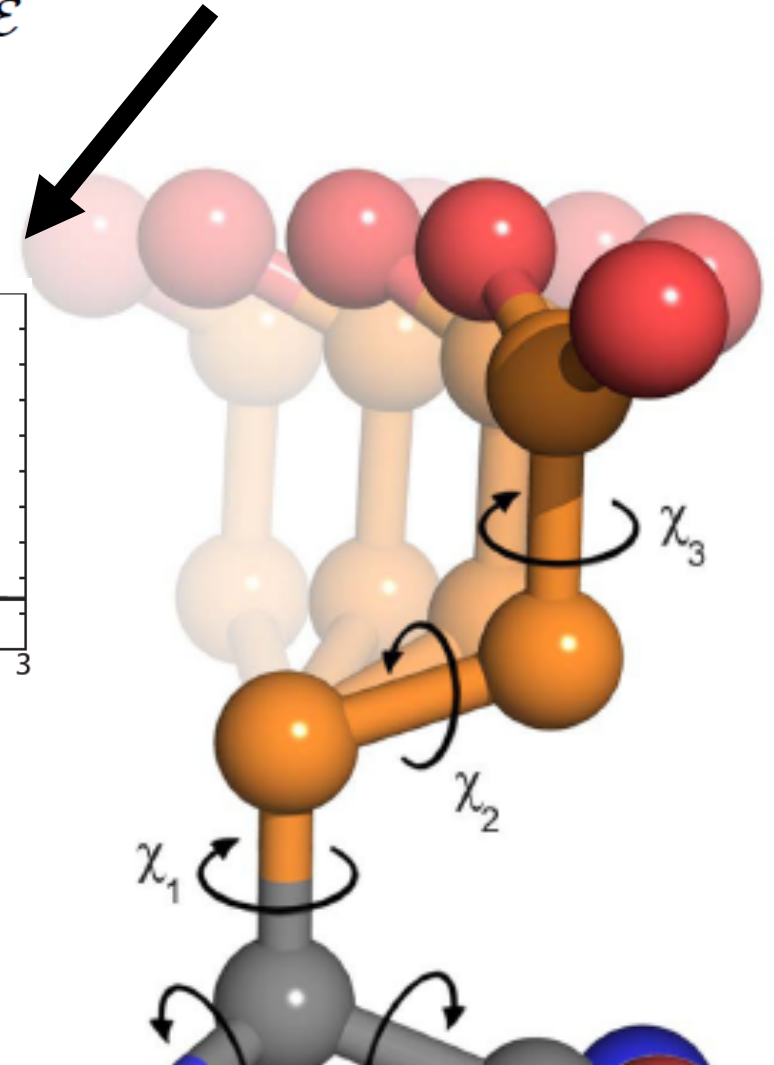
Rotamer Likelihood



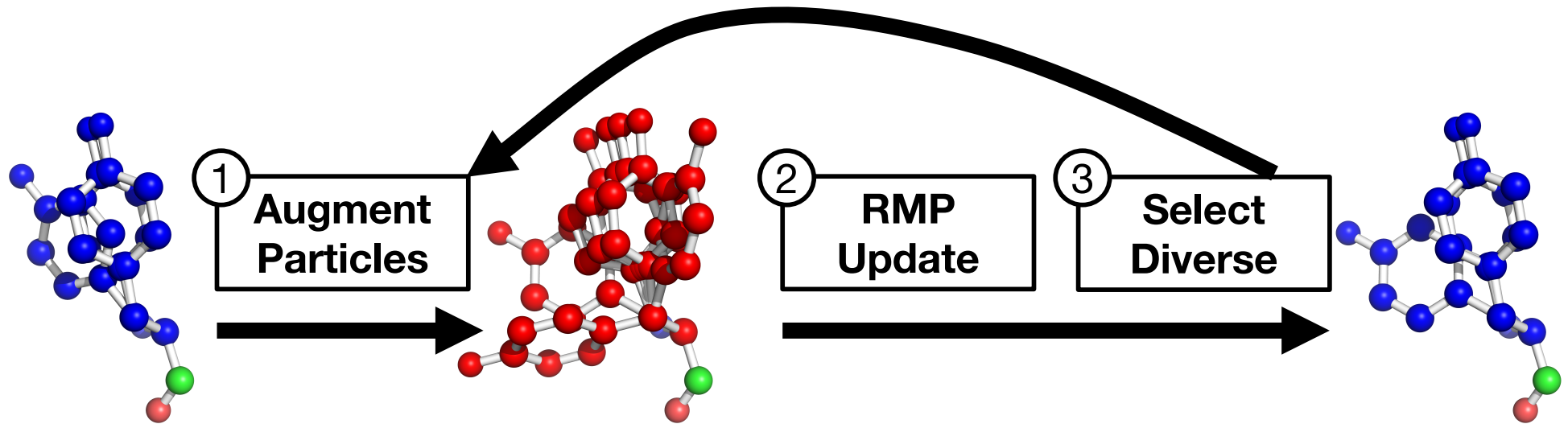
Atomic Interaction



Statistical and physical potential functions.

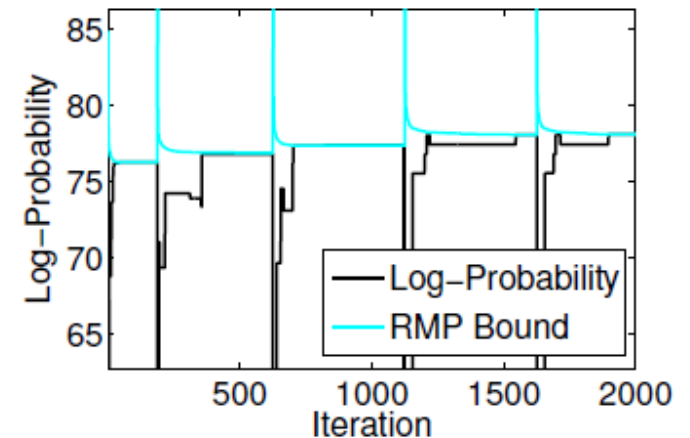


# D-PMP for Side Chains

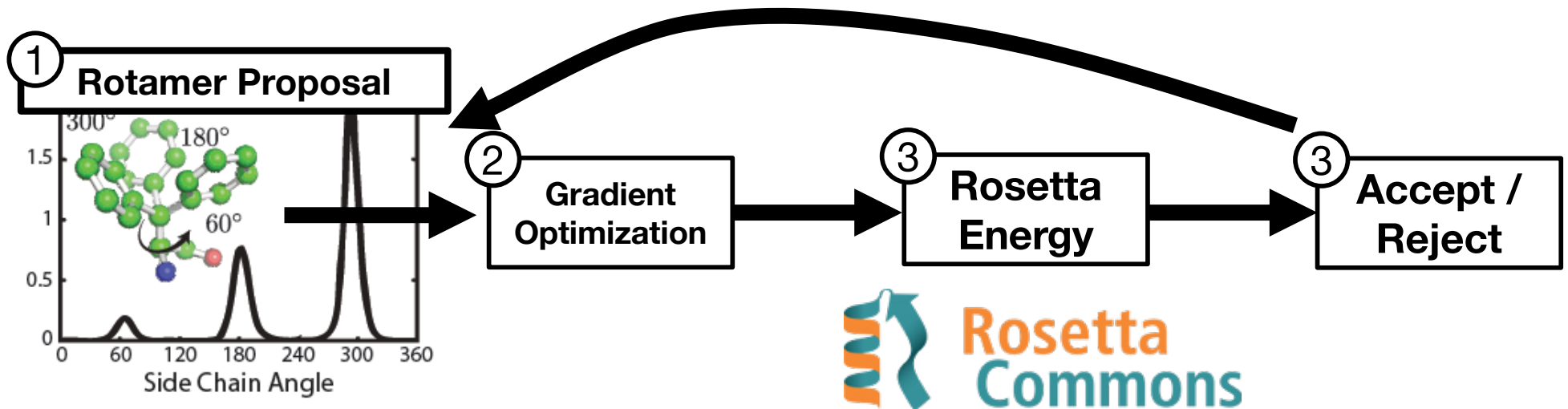


Continuous optimization of side chains:

- Captures non-rotameric side chains
- Conformational diversity
- Likelihood-based proposals



# Rosetta



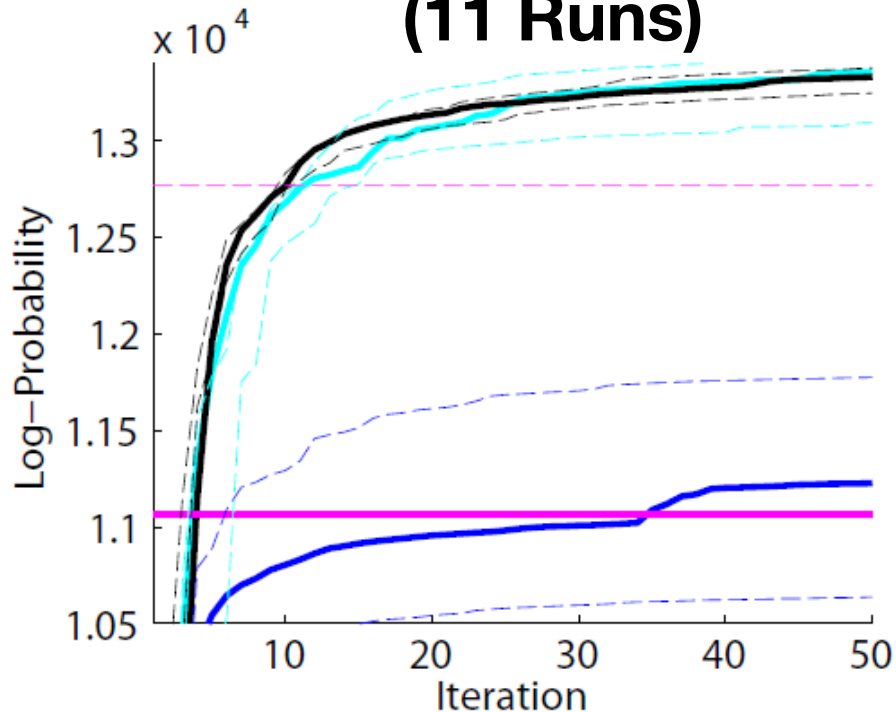
- Energy model used in FoldIt game
- Simulated annealing (SA) Monte Carlo
- Independent chains for multiple optima

**Replace SA with D-PMP. Use Rosetta as black-box energy method.**

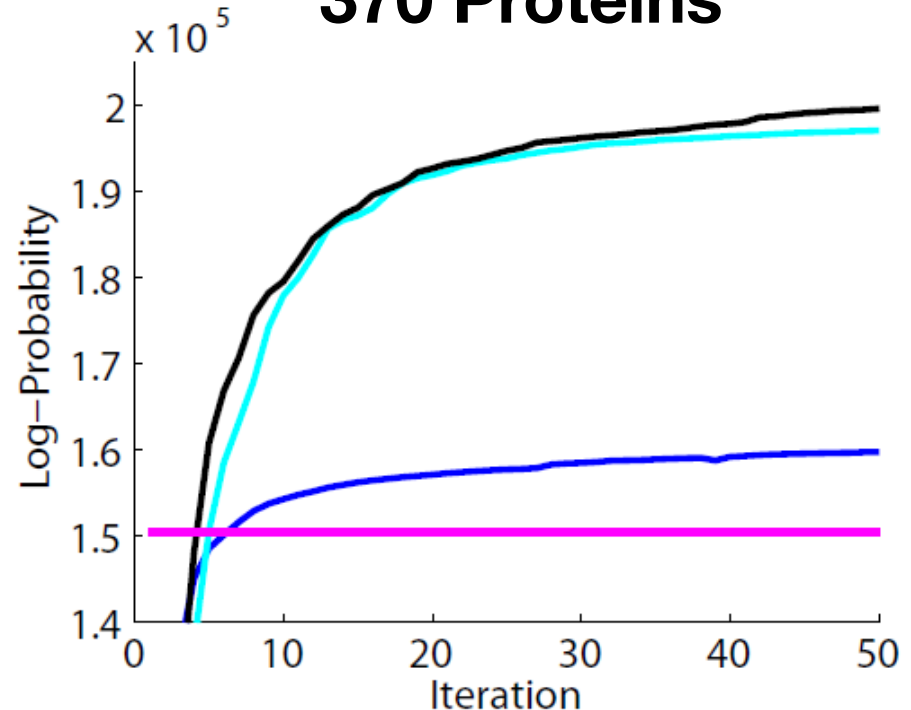
# Protein Side Chain Prediction

Log-probability of MAP estimate for...

**20 Proteins  
(11 Runs)**



**370 Proteins**

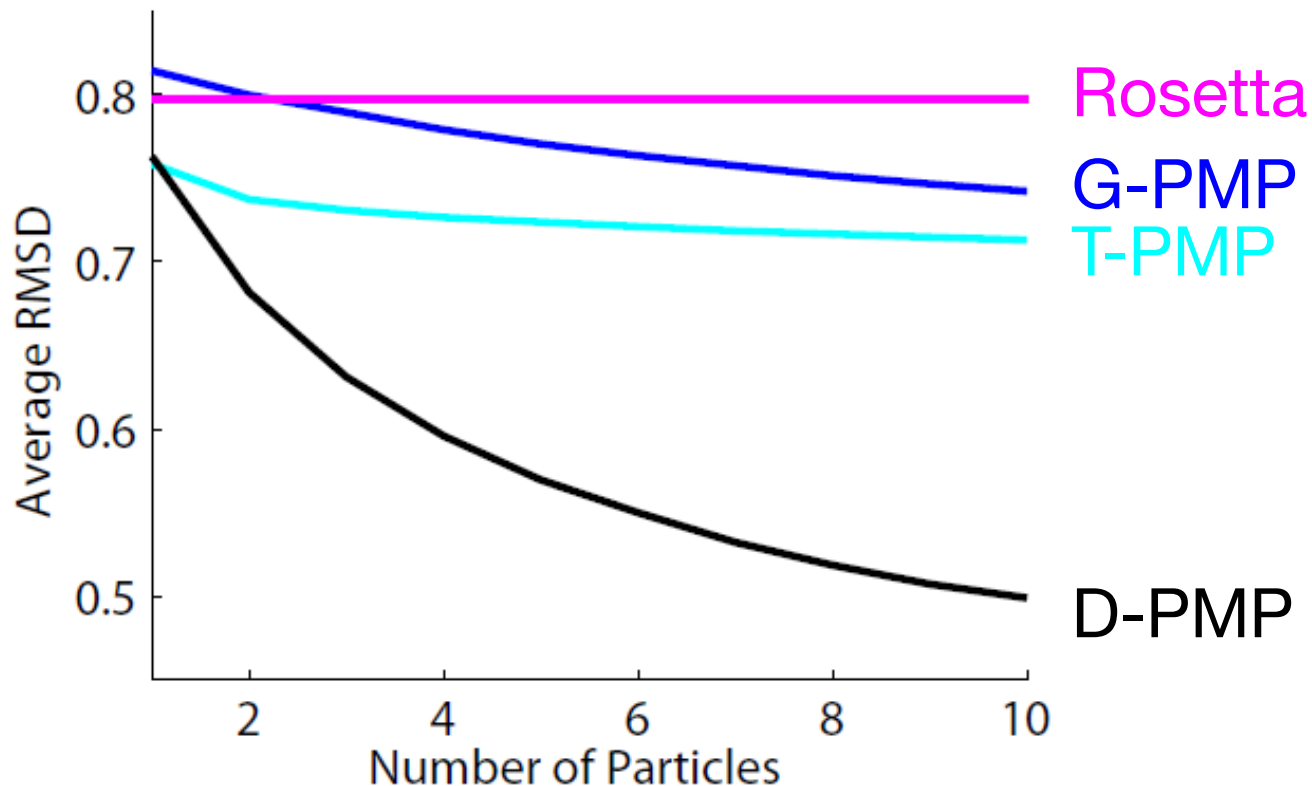


**G-PMP, T-PMP, D-PMP, Rosetta** simulated annealing [Rohl et al., 2004]



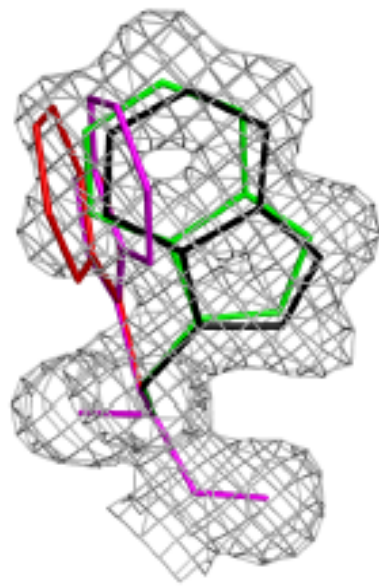
# Protein Side Chain Prediction

Root mean square deviation (RMSD)  
from x-ray structure.

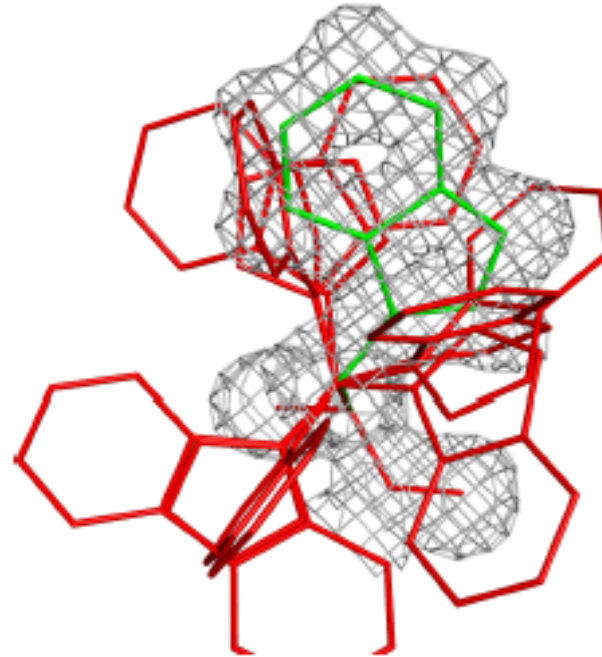


Oracle selects best configuration in  
current particle set.

# Non-Rotameric Side Chains



Estimate



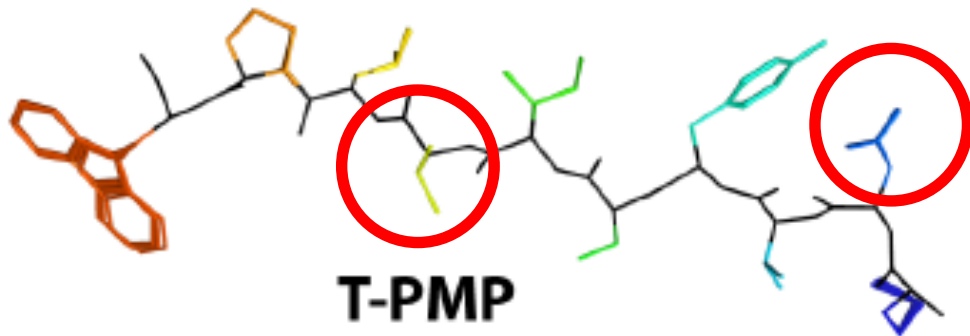
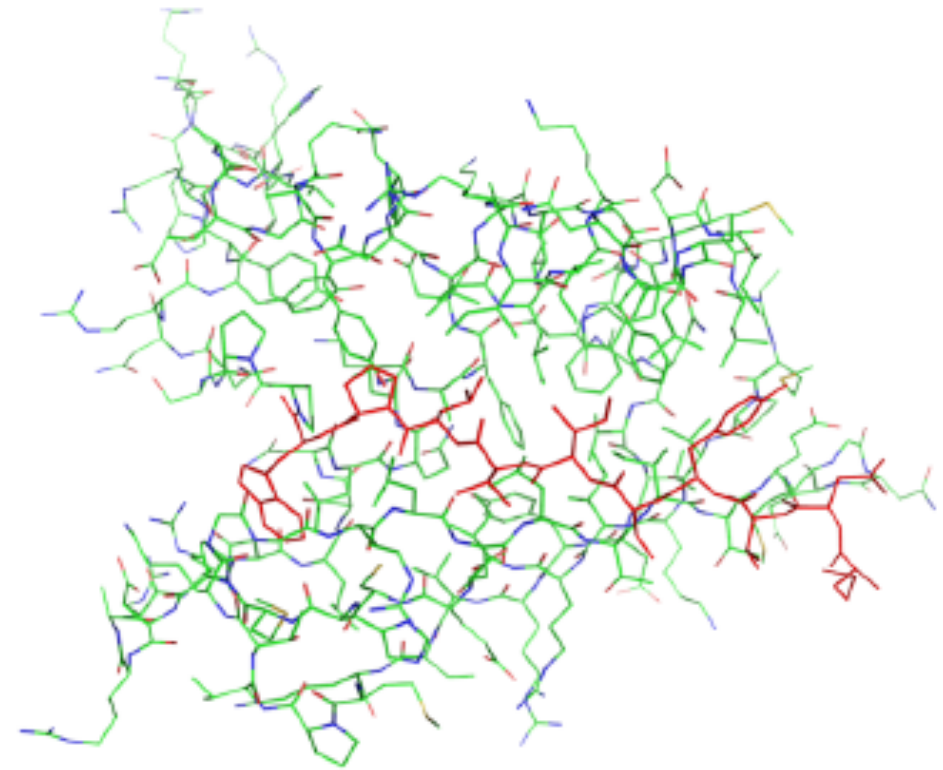
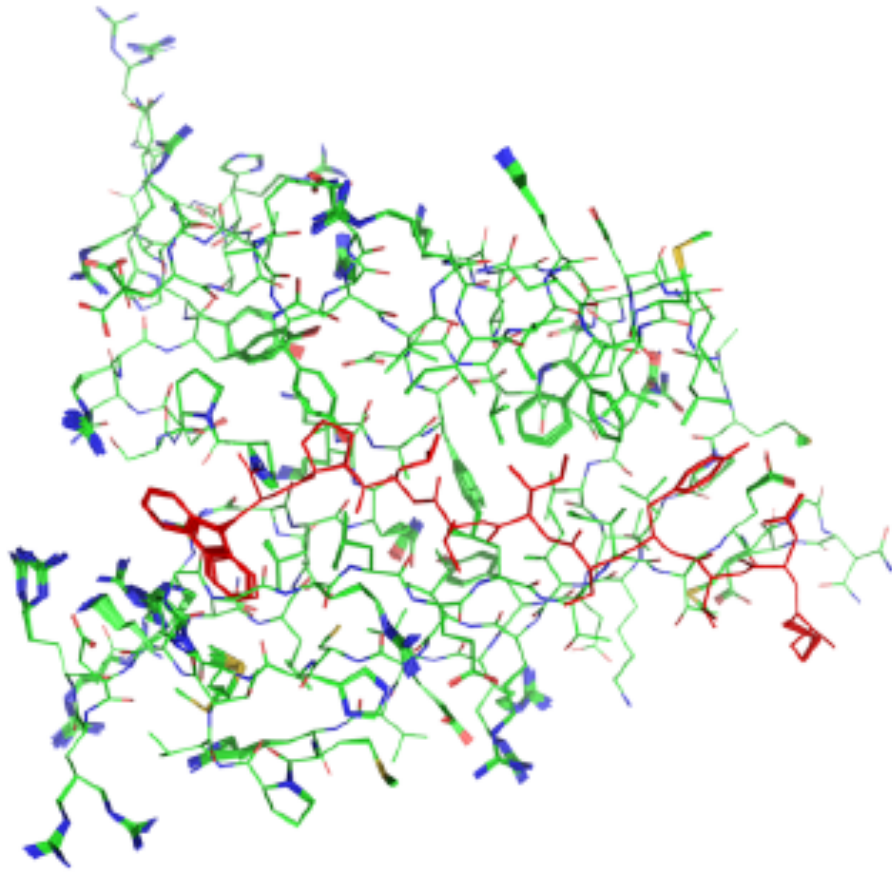
Rotamers



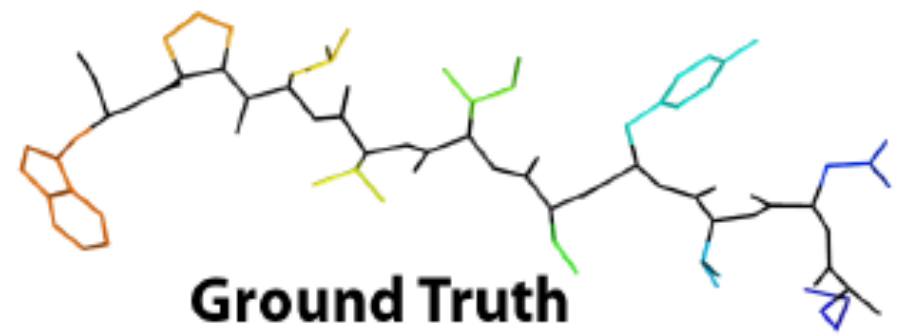
D-PMP Particles

Not all side chains obey standard rotamer discretization.

# Protein Side Chain Prediction

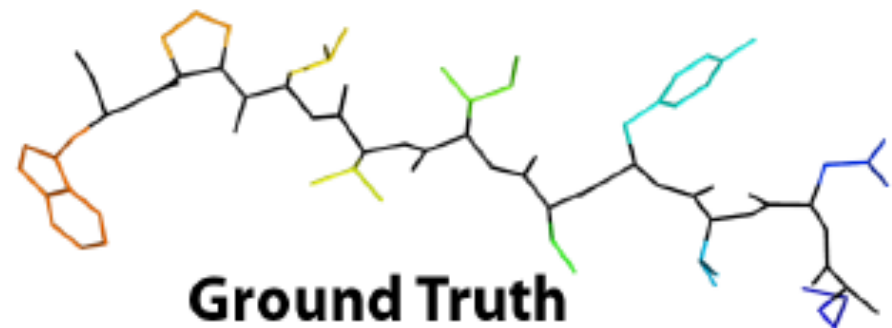
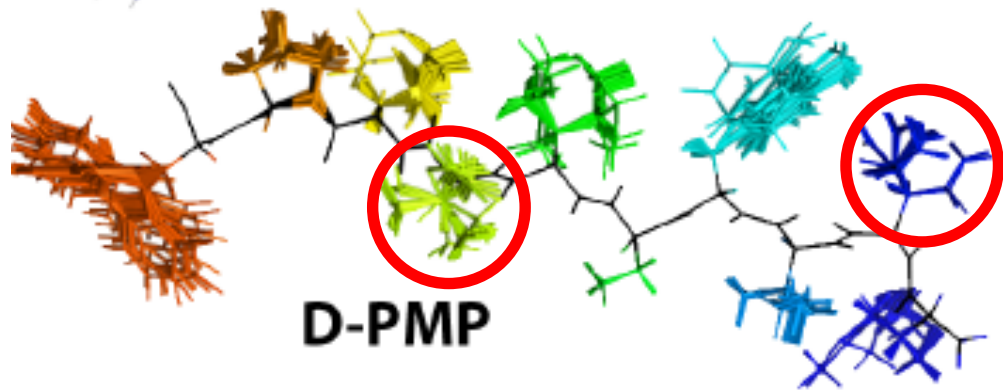
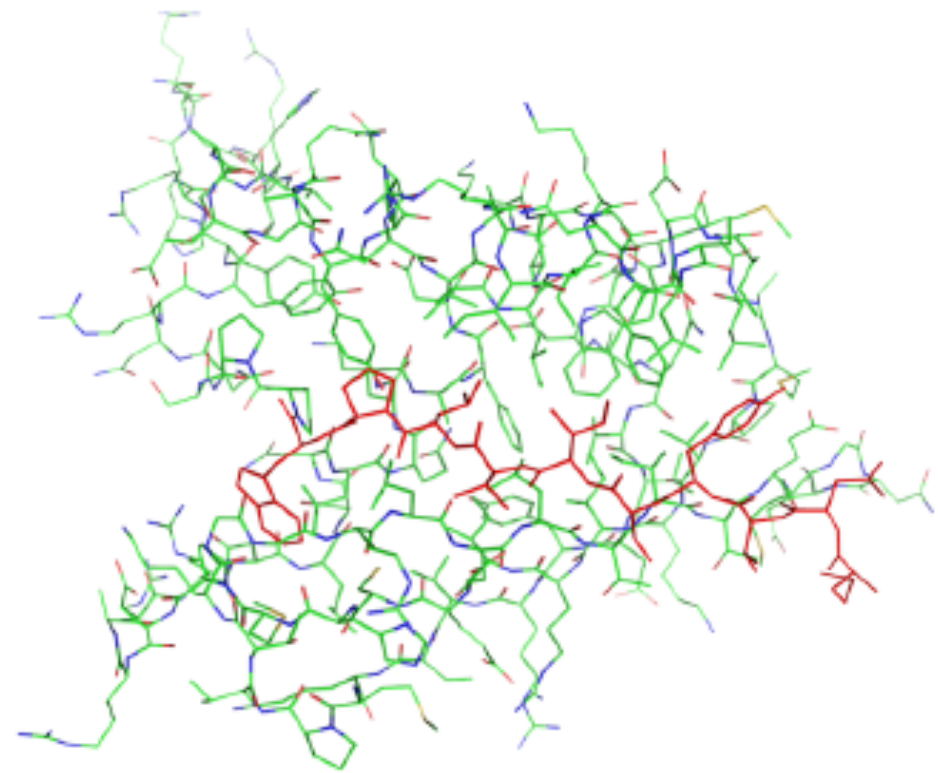
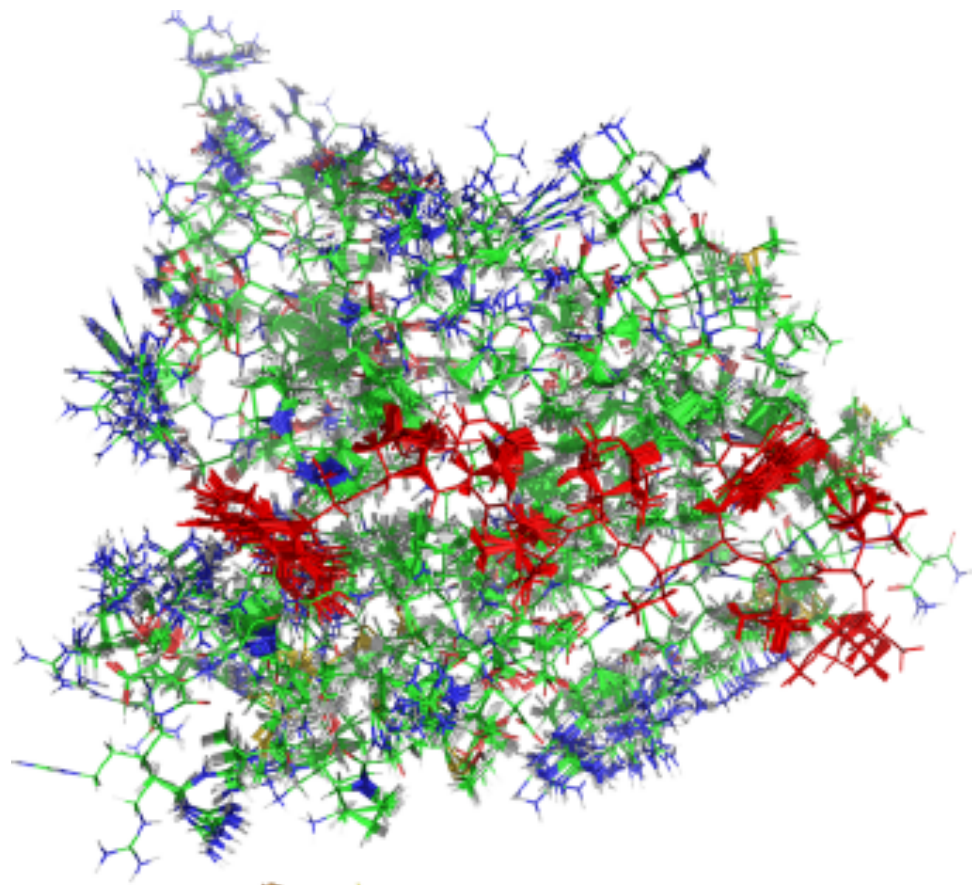


**T-PMP**



**Ground Truth**

# Protein Side Chain Prediction



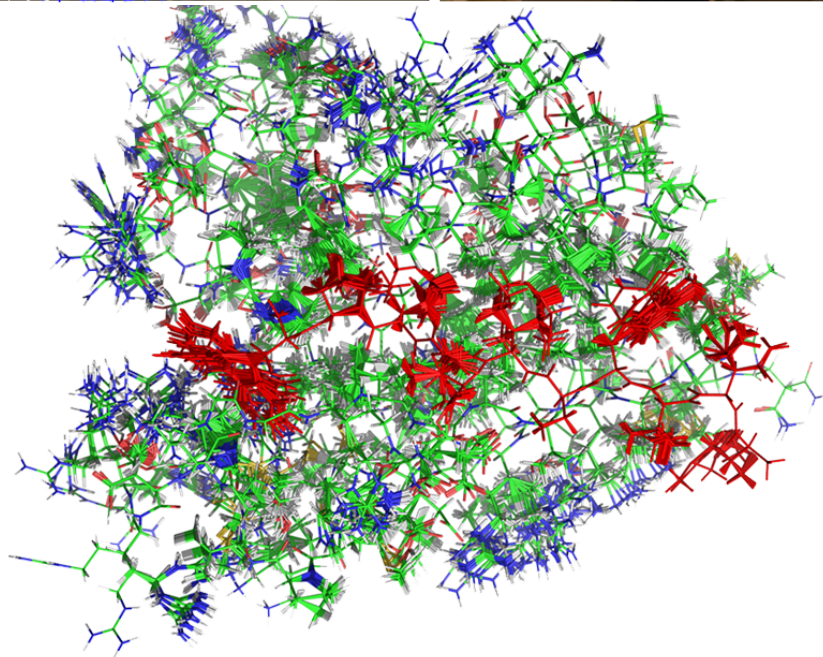


# Contributions

**Reliable particle-based MAP inference**  
for graphical models with continuous variables:  
*object shape, articulation, position, motion, ...*



**Validation:** *Inference of multiple poses, motions, protein conformations, ...*



**Guarantees of Reliability:**  
*Rigorous, non-asymptotic bounds on accuracy of diverse particle selection*

**Code:** *General-purpose, black-box inference for continuous graphical models*