# Iterative closest point registration

Jan Kybic

2020

*Besl, McKey: A method for registration of 3D shapes. 1992*

## Key points:

- Find a geometric transformation between two point sets or a point set and a parametric model
- Matching closest points
- Iterative
- Rigid transformations (extensions possible)

# 3D Example

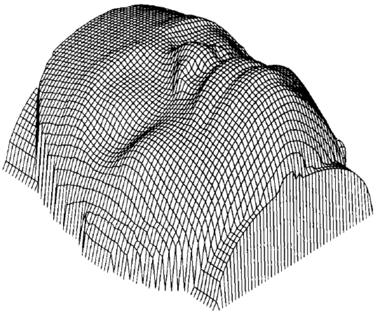
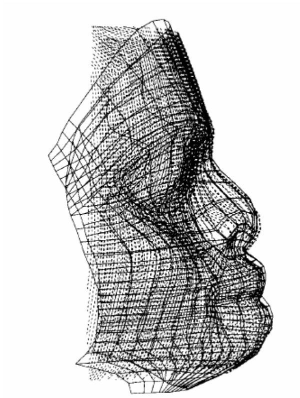


Fig. 12. Model surface: Range image of mask: 8442 triangles.



# Geometric models

- Points
- Lines
- Triangles
- Parametric models
- Implicit models

## Finding distance

- closed form
- iteratively (e.g. Newton method

# Quaternions for rotation representation

- "Four-vector"
  $\mathbf{q}=(q_0, q_1, q_2, q_3) = q_0 + iq_1 + jq_2 + kq_3 = q_0 + (q_1, q_2, q_3)$, with
  $i^2 = j^2 = k^2 = -1$
- Rotation by angle $\alpha$ around axis $\mathbf{u}$

$$\mathbf{q}=\cos\frac{\alpha}{2} + \mathbf{u}\sin\frac{\alpha}{2} = \left(\cos\frac{\alpha}{2}, u_x\sin\frac{\alpha}{2}, u_y\sin\frac{\alpha}{2}, u_z\sin\frac{\alpha}{2}\right)$$

- Applying a rotation

$\mathbf{Rv}=\mathbf{q}\ \mathbf{v}\ \mathbf{q}^{-1}$ with $\boldsymbol{q}^{-1} = \frac{(q_0, -q_1, -q_2, -q_3)}{q_0^2+q_1^2+q_2^2+q_3^2}$

- Rotation matrix from a unit quaternion ($q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$)

$$\boldsymbol{R} = \begin{bmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2(q_1q_2-q_0q_3) & 2(q_1q_3+q_0q_2) \\ 2(q_1q_2+q_0q_3) & q_0^2+q_2^2-q_1^2-q_3^2 & 2(q_2q_3-q_0q_1) \\ 2(q_1q_3-q_0q_2) & 2(q_2q_3+q_0q_1) & q_0^2+q_3^2-q_1^2-q_2^2 \end{bmatrix}$$

# Closed-form for rotation and translation

The unit quaternion is a four vector $\vec{q}_R = [q_0 q_1 q_2 q_3]^t$, where $q_0 \geq 0$, and $q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$. The $3 \times 3$ rotation matrix generated by a unit rotation quaternion is found at the bottom of this page. Let $\vec{q}_T = [q_4 q_5 q_6]^t$ be a translation vector. The complete registration state vector $\vec{q}$ is denoted $\vec{q} = [\vec{q}_R | \vec{q}_T]^t$. Let $P = \{\vec{p}_i\}$ be a measured data point set to be aligned with a model point set $X = \{\vec{x}_i\}$, where $N_x = N_p$ and where each point $\vec{p}_i$ corresponds to the point $\vec{x}_i$ with the same index. The mean square objective function to be minimized is

$$f(\vec{q}\,) = \frac{1}{N_p} \sum_{i=1}^{N_p} \| \vec{x}_i - \boldsymbol{R}(\vec{q}_R)\vec{p}_i - \vec{q}_T \|^2. \qquad (22)$$

# Closed-form for rotation and translation (2)

The "center of mass" $\vec{\mu}_p$ of the measured point set $P$ and the center of mass $\vec{\mu}_x$ for the $X$ point set are given by

$$\vec{\mu}_p = \frac{1}{N_p}\sum_{i=1}^{N_p}\vec{p}_i \quad \text{and} \quad \vec{\mu}_x = \frac{1}{N_x}\sum_{i=1}^{N_x}\vec{x}_i. \qquad (23)$$

The cross-covariance matrix $\Sigma_{px}$ of the sets $P$ and $X$ is given by

$$\Sigma_{px} = \frac{1}{N_p}\sum_{i=1}^{N_p}[(\vec{p}_i - \vec{\mu}_p)(\vec{x}_i - \vec{\mu}_x)^t] = \frac{1}{N_p}\sum_{i=1}^{N_p}[\vec{p}_i\vec{x}_i^t] - \vec{\mu}_p\vec{\mu}_x^{\,t}.$$

# Closed-form for rotation and translation (3)

The cyclic components of the anti-symmetric matrix $A_{ij} = (\Sigma_{px} - \Sigma_{px}^T)_{ij}$ are used to form the column vector $\Delta = [A_{23} \quad A_{31} \quad A_{12}]^T$. This vector is then used to form the symmetric $4 \times 4$ matrix $Q(\Sigma_{px})$

$$Q(\Sigma_{px}) = \begin{bmatrix} \mathrm{tr}(\Sigma_{px}) & \Delta^T \\ \Delta & \Sigma_{px} + \Sigma_{px}^T - \mathrm{tr}(\Sigma_{px})\boldsymbol{I}_3 \end{bmatrix} \tag{25}$$

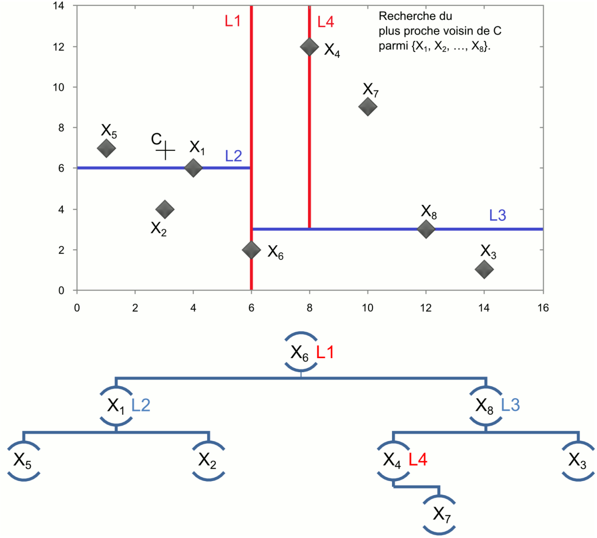
where $\boldsymbol{I}_3$ is the $3 \times 3$ identity matrix. The unit eigenvector $\vec{q}_R = [q_0 \quad q_1 \quad q_2 \quad q_3]^t$ corresponding to the maximum eigenvalue of the matrix $Q(\Sigma_{px})$ is selected as the optimal rotation. The optimal translation vector is given by

$$\vec{q}_T = \vec{\mu}_x - \boldsymbol{R}(\vec{q}_R)\vec{\mu}_p. \tag{26}$$

Horn, Closed-form solution of absolute orientation using unit quaternions. J.Opt. Soc. Amer., 1987

# Finding closest points

- Brute force $O(N_p N_x)$
- Grid method, k-D tree, $O(N_p \log N_x)$ on the average




- Approximate nearest neighbors

# Iterative closest point algorithm

Initialize **q** as identity, $P_0 = P$. Repeat:

a. Compute the closest points: $Y_k = \mathcal{C}(P_k, X)$ (cost: $0(N_p N_x)$ worst case, $0(N_p \log N_x)$ average).

b. Compute the registration: $(\vec{q}_k, d_k) = \mathcal{Q}(P_0, Y_k)$ (cost: $O(N_p)$).

c. Apply the registration: $P_{k+1} = \vec{q}_k(P_0)$ (cost: $O(N_p)$).

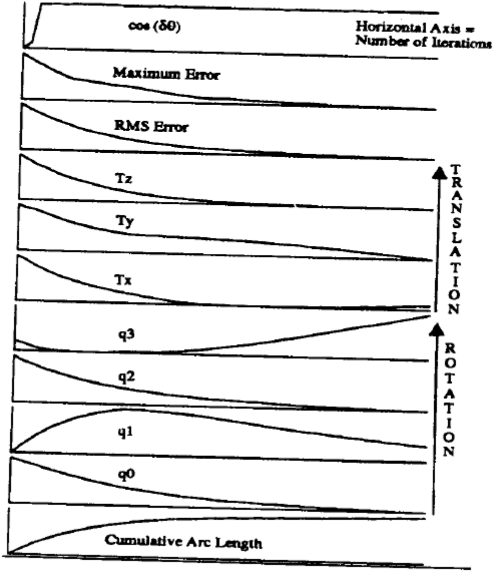
d. Terminate the iteration when the change in mean-square error falls below a preset threshold $\tau > 0$ specifying the desired precision of the registration: $d_k - d_{k+1} < \tau$.

# ICP convergence

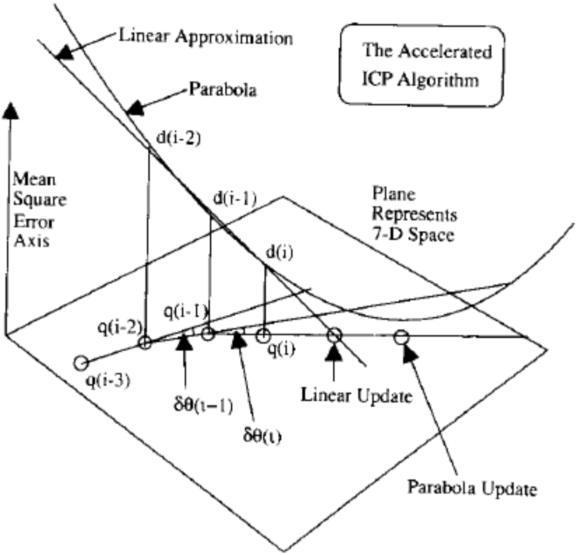
and proved. The key ideas are that 1) least squares registration generically reduces the average distance between corresponding points during each iteration, whereas 2) the closest point determination generically reduces the distance for each point individually. Of course, this individual distance reduction also reduces the average distance because the average of a set of smaller positive numbers is smaller. We offer a more elaborate explanation in the proof below.

*Theorem:* The iterative closest point algorithm always converges monotonically to a local minimum with respect to the mean-square distance objective function.

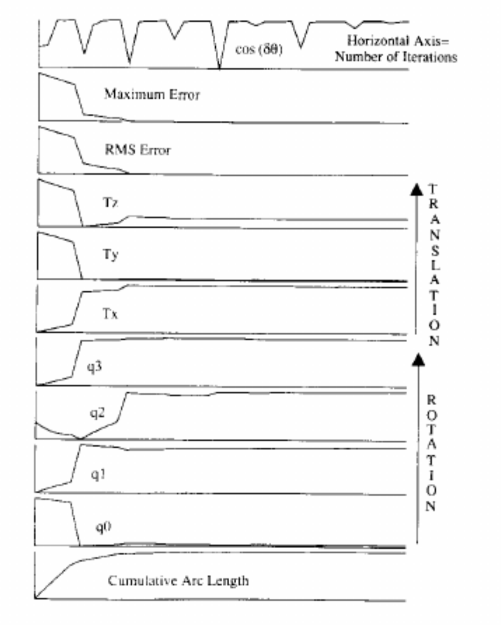
# Parameter evolution



# Accelerated ICP



# Accelerated parameter evolution



# Initial pose estimation

- ICP finds only **local minima**, sensitive to initial pose
- If sufficient overlap $\rightarrow$ not too sensitive to translation
- Uniform/random sampling of initial poses

## Moment matching

- align centers of gravity
- calculate covariance matrices
- find and match eigenvectors
- rotate to align eigenvectors

# Conclusions

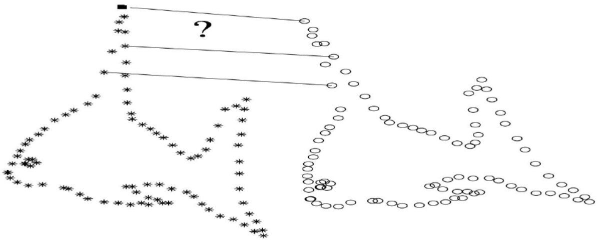
- Simple and fast method for matching 2D/3D shapes or point sets
- Needs good initialization
- Sufficient overlap
- Widely used in practice
- Many extensions to make it more robust (e.g. ICRP, soft assignment)

*Myronenko, Song: Point Set Registration: Coherent Point Drift 2010*

## Key points:

- Probabilistic extension to ICP
- Both rigid and nonrigid registration
- Gaussian density model
- Soft assignment
- Can handle outliers

# Example point set registration problem



# Probabilistic model

We consider the points in $\mathbf{Y}$ as the GMM centroids and the points in $\mathbf{X}$ as the data points generated by the GMM. The GMM probability density function is

$$p(\mathbf{x}) = \sum_{m=1}^{M+1} P(m)p(\mathbf{x}|m), \tag{1}$$

where $p(\mathbf{x}|m) = \frac{1}{(2\pi\sigma^2)^{D/2}} \exp^{-\frac{\|\mathbf{x}-\mathbf{y}_m\|^2}{2\sigma^2}}$. We also added an additional uniform distribution $p(\mathbf{x}|M+1) = \frac{1}{N}$ to the mixture model to account for noise and outliers. We use equal isotropic covariances $\sigma^2$ and equal membership probabilities $P(m) = \frac{1}{M}$ for all GMM components

# Probabilistic model (2)

$(m = 1, \ldots, M)$. Denoting the weight of the uniform distribution as $w$, $0 \leq w \leq 1$, the mixture model takes the form

$$p(\mathbf{x}) = w \frac{1}{N} + (1 - w) \sum_{m=1}^{M} \frac{1}{M} p(\mathbf{x}|m). \qquad (2)$$

We reparameterize the GMM centroid locations by a set of parameters $\theta$ and estimate them by maximizing the likelihood or, equivalently, by minimizing the negative log-likelihood function

$$E(\theta, \sigma^2) = -\sum_{n=1}^{N} \log \sum_{m=1}^{M+1} P(m) p(\mathbf{x}_n|m), \qquad (3)$$

where we make the i.i.d. data assumption. We define the

Centroid locations $y(\theta)$

# EM algorithm

- Find $\theta$,$\sigma^2$by alternative maximization of $E$
- **Expectation** step calculates posterior prob. of $y_m$given $x_n$for fixed $\theta, \sigma^2$

$$P(m|\mathbf{x}_n) = P(m)p(\mathbf{x}_n|m)/p(\mathbf{x}_n)$$

- **Maximization** step minimizes the expected negative log-likelihood $Q = \mathrm{E}[\log P(\theta, \sigma|X, Y)] \geq E$ for fixed $P^{\mathrm{old}}(m|x_n)$

$$Q = -\sum_{n=1}^{N}\sum_{m=1}^{M+1} P^{old}(m|\mathbf{x}_n)\log(P^{new}(m)p^{new}(\mathbf{x}_n|m)),$$

# Minimization of Q

$$Q(\theta, \sigma^2) = \frac{1}{2\sigma^2} \sum_{n=1}^{N} \sum_{m=1}^{M} P^{\text{old}}(m|\mathbf{x}_n) \|\mathbf{x}_n - \mathcal{T}(\mathbf{y}_m, \theta)\|^2 + \frac{N_{\mathbf{P}} D}{2} \log \sigma^2,$$

$$P^{old}(m|\mathbf{x}_n) = \frac{\exp^{-\frac{1}{2}\left\| \frac{\mathbf{x}_n - \mathcal{T}(\mathbf{y}_m, \theta^{old})}{\sigma^{old}} \right\|^2}}{\sum_{k=1}^{M} \exp^{-\frac{1}{2}\left\| \frac{\mathbf{x}_n - \mathcal{T}(\mathbf{y}_k, \theta^{old})}{\sigma^{old}} \right\|^2} + c},$$

# Rigid and affine transformations

$$Q(\mathbf{R}, \mathbf{t}, s, \sigma^2) = \frac{1}{2\sigma^2} \sum_{m,n=1}^{M,N} P^{\text{old}}(m|\mathbf{x}_n) \|\mathbf{x}_n - s\mathbf{R}\mathbf{y}_m - \mathbf{t}\|^2 + \frac{N_{\mathbf{P}} D}{2} \log \sigma^2, \quad \text{s.t. } \mathbf{R}^T\mathbf{R} = \mathbf{I}, \; \det(\mathbf{R}) = 1.$$

Can be minimized analytically for $\mathbf{R}$, $\mathbf{t}$, $s$, $\sigma^2$. $\boldsymbol{R}$ is found using SVD.

# Rigid coherent point drift

**Rigid point set registration algorithm:**

- Initialization: $\mathbf{R} = \mathbf{I}, \mathbf{t} = 0, s = 1, 0 \leq w \leq 1$

  $\sigma^2 = \frac{1}{DNM} \sum_{n=1}^{N} \sum_{m=1}^{M} \|\mathbf{x}_n - \mathbf{y}_m\|^2$
- EM optimization, repeat until convergence:
  - E-step: Compute $\mathbf{P}$,

    $$p_{mn} = \frac{\exp^{-\frac{1}{2\sigma^2}\|\mathbf{x}_n - (s\mathbf{R}\mathbf{y}_m + \mathbf{t})\|^2}}{\sum_{k=1}^{M} \exp^{-\frac{1}{2\sigma^2}\|\mathbf{x}_n - (s\mathbf{R}\mathbf{y}_k + \mathbf{t})\|^2} + (2\pi\sigma^2)^{D/2} \frac{w}{1-w} \frac{M}{N}}$$
  - M-step: Solve for $\mathbf{R}, s, \mathbf{t}, \sigma^2$:
    - $N_{\mathbf{P}} = \mathbf{1}^T \mathbf{P} \mathbf{1}, \mu_{\mathbf{x}} = \frac{1}{N_{\mathbf{P}}} \mathbf{X}^T \mathbf{P}^T \mathbf{1}, \mu_{\mathbf{y}} = \frac{1}{N_{\mathbf{P}}} \mathbf{Y}^T \mathbf{P} \mathbf{1},$
    - $\hat{\mathbf{X}} = \mathbf{X} - \mathbf{1}\mu_{\mathbf{x}}^T, \ \hat{\mathbf{Y}} = \mathbf{Y} - \mathbf{1}\mu_{\mathbf{y}}^T,$
    - $\mathbf{A} = \hat{\mathbf{X}}^T \mathbf{P}^T \hat{\mathbf{Y}}$, compute SVD of $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$,
    - $\mathbf{R} = \mathbf{U}\mathbf{C}\mathbf{V}^T$, where $\mathbf{C} = \mathrm{d}(1, .., 1, \det(\mathbf{U}\mathbf{V}^T))$,
    - $s = \frac{\mathrm{tr}(\mathbf{A}^T \mathbf{R})}{\mathrm{tr}(\hat{\mathbf{Y}}^T \mathrm{d}(\mathbf{P}\mathbf{1})\hat{\mathbf{Y}})},$
    - $\mathbf{t} = \mu_{\mathbf{x}} - s\mathbf{R}\mu_{\mathbf{y}},$
    - $\sigma^2 = \frac{1}{N_{\mathbf{P}} D} (\mathrm{tr}(\hat{\mathbf{X}}^T \mathrm{d}(\mathbf{P}^T \mathbf{1}) \hat{\mathbf{X}}) - s \, \mathrm{tr}(\mathbf{A}^T \mathbf{R})).$
- The aligned point set is $\mathcal{T}(\mathbf{Y}) = s\mathbf{Y}\mathbf{R}^T + \mathbf{1}\mathbf{t}^T$,
- The probability of correspondence is given by $\mathbf{P}$.

# Affine coherent point drift

**Affine point set registration algorithm:**

- Initialization: $\mathbf{B} = \mathbf{I}, \mathbf{t} = 0, 0 \leq w \leq 1$
  $\sigma^2 = \frac{1}{DNM} \sum_{n=1}^{N} \sum_{m=1}^{M} \|\mathbf{x}_n - \mathbf{y}_m\|^2$
- EM optimization, repeat until convergence:
  - E-step: Compute $\mathbf{P}$,
    $$p_{mn} = \frac{\exp^{-\frac{1}{2\sigma^2}\|\mathbf{x}_n - (\mathbf{B}\mathbf{y}_m + \mathbf{t})\|^2}}{\sum_{k=1}^{M} \exp^{-\frac{1}{2\sigma^2}\|\mathbf{x}_n - (\mathbf{B}\mathbf{y}_k + \mathbf{t})\|^2} + (2\pi\sigma^2)^{D/2} \frac{w}{1-w} \frac{M}{N}}$$
  - M-step: Solve for $\mathbf{B}, \mathbf{t}, \sigma^2$:
    - $\cdot\ N_{\mathbf{P}} = \mathbf{1}^T \mathbf{P} \mathbf{1}, \mu_{\mathbf{x}} = \frac{1}{N_{\mathbf{P}}} \mathbf{X}^T \mathbf{P}^T \mathbf{1}, \mu_{\mathbf{y}} = \frac{1}{N_{\mathbf{P}}} \mathbf{Y}^T \mathbf{P} \mathbf{1},$
    - $\cdot\ \hat{\mathbf{X}} = \mathbf{X} - \mathbf{1}\mu_{\mathbf{x}}^T,\ \hat{\mathbf{Y}} = \mathbf{Y} - \mathbf{1}\mu_{\mathbf{y}}^T,$
    - $\cdot\ \mathbf{B} = (\hat{\mathbf{X}}^T \mathbf{P}^T \hat{\mathbf{Y}})(\hat{\mathbf{Y}}^T \mathrm{d}(\mathbf{P}\mathbf{1})\hat{\mathbf{Y}})^{-1},$
    - $\cdot\ \mathbf{t} = \mu_{\mathbf{x}} - \mathbf{B}\mu_{\mathbf{y}},$
    - $\cdot\ \sigma^2 = \frac{1}{N_{\mathbf{P}} D}(\mathrm{tr}(\hat{\mathbf{X}}^T \mathrm{d}(\mathbf{P}^T \mathbf{1})\hat{\mathbf{X}}) - \mathrm{tr}(\hat{\mathbf{X}}^T \mathbf{P}^T \hat{\mathbf{Y}} \mathbf{B}^T)).$
- The aligned point set is $\mathcal{T}(\mathbf{Y}) = \mathbf{Y}\mathbf{B}^T + 1\mathbf{t}^T$,
- The probability of correspondence is given by $\mathbf{P}$.

# Nonrigid registration

- Variational formulation with a smoothness regularization term

$$\mathcal{T}(\mathbf{Y}, v) = \mathbf{Y} + v(\mathbf{Y}). \qquad f(v, \sigma^2) = E(v, \sigma^2) + \frac{\lambda}{2}\phi(v),$$

$$\|v\|^2_{\mathbb{H}^m} = \int_{\mathbb{R}} \sum_{k=0}^{m} \left\| \frac{\partial^k v}{\partial x^k} \right\|^2 dx. \qquad \phi(v) = \|v\|^2_{\mathbb{H}^m} = \|Lv\|^2,$$

- Minimizing

$$Q(v, \sigma^2) = \frac{1}{2\sigma^2} \sum_{m,n=1}^{M,N} P^{\text{old}}(m|\mathbf{x}_n) \|\mathbf{x}_n - (\mathbf{y}_m + v(\mathbf{y}_m))\|^2 + \frac{N_{\mathbf{P}} D}{2} \log \sigma^2 + \frac{\lambda}{2} \|Lv\|^2.$$

- Solution must have the form (from Euler-Lagrange equations) with a Green's function $\hat{L}LG = \delta$

$$v(\mathbf{z}) = \sum_{m=1}^{M} \mathbf{w}_m G(\mathbf{z}, \mathbf{y}_m) + \psi(\mathbf{z}),$$

# Regularization term

$$\phi(v) = \int_{\mathbb{R}^D} \frac{|\tilde{v}(\mathbf{s})|^2}{\tilde{G}(\mathbf{s})}\, d\mathbf{s}, \qquad \phi_{MCT}(v) = \int_{\mathbb{R}^d} \sum_{l=0}^{\infty} \frac{\beta^{2l}}{l!2^l} \left\| D^l v(\mathbf{x}) \right\|^2 d\mathbf{x},$$

- Green's function is a Gaussian
- Coefficients **w** minimizing Q found by

$$(\mathbf{G} + \lambda\sigma^2 d(\mathbf{P1})^{-1})\mathbf{W} = d(\mathbf{P1})^{-1}\mathbf{PX} - \mathbf{Y}$$

# Non-rigid coherent point drift

**Non-rigid point set registration algorithm:**

- Initialization: $\mathbf{W} = 0, \sigma^2 = \frac{1}{DNM} \sum_{m,n=1}^{M,N} \|\mathbf{x}_n - \mathbf{y}_m\|^2$
- Initialize $w (0 \leq w \leq 1)$, $\beta > 0$, $\lambda > 0$,
- Construct $\mathbf{G}$: $g_{ij} = \exp^{-\frac{1}{2\beta^2}\|\mathbf{y}_i - \mathbf{y}_j\|^2}$,
- EM optimization, repeat until convergence:
  - E-step: Compute $\mathbf{P}$,

$$p_{mn} = \frac{\exp^{-\frac{1}{2\sigma^2}\|\mathbf{x}_n - (\mathbf{y}_m + \mathbf{G}(m,\cdot)\mathbf{W})\|^2}}{\sum_{k=1}^{M} \exp^{-\frac{1}{2\sigma^2}\|\mathbf{x}_n - (\mathbf{y}_k + \mathbf{G}(k,\cdot)\mathbf{W})\|^2} + \frac{w}{1-w}\frac{(2\pi\sigma^2)^{D/2} M}{N}}$$

  - M-step:
    - Solve $(\mathbf{G} + \lambda\sigma^2 d(\mathbf{P1})^{-1})\mathbf{W} = d(\mathbf{P1})^{-1}\mathbf{PX} - \mathbf{Y}$
    - $N_{\mathbf{P}} = \mathbf{1}^T\mathbf{P1}$, $\mathbf{T} = \mathbf{Y} + \mathbf{GW}$,
    - $\sigma^2 = \frac{1}{N_{\mathbf{P}} D}(\mathrm{tr}(\mathbf{X}^T \mathrm{d}(\mathbf{P}^T\mathbf{1})\mathbf{X}) - 2\,\mathrm{tr}((\mathbf{PX})^T\mathbf{T}) + \mathrm{tr}(\mathbf{T}^T \mathrm{d}(\mathbf{P1})\mathbf{T}))$,
- The aligned point set is $\mathbf{T} = \mathcal{T}(\mathbf{Y}, \mathbf{W}) = \mathbf{Y} + \mathbf{GW}$,
- The probability of correspondence is given by $\mathbf{P}$.

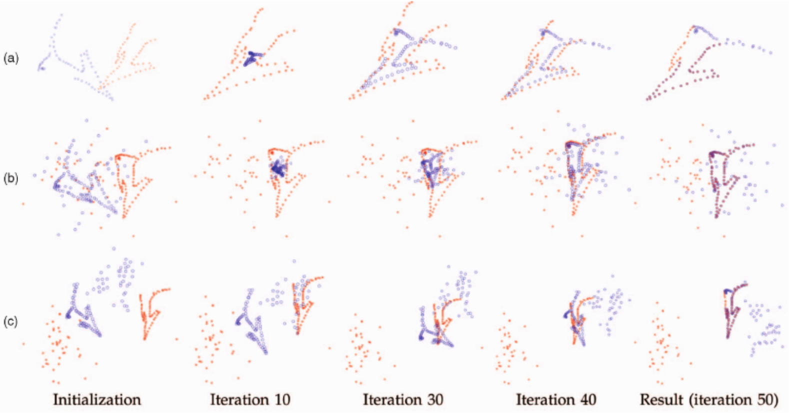
# CPD algorithm notes

- Three parameters: $w$,$\lambda$,$\beta$
- Alternative minimization of $\sigma^2$and $\boldsymbol{W}$, very few iterations needed

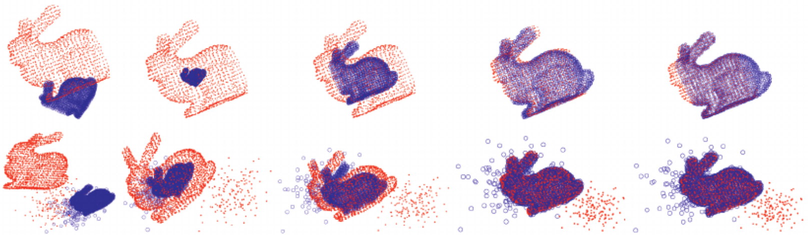
## Speed

- Complexity $O(NM + M^3)$per iteration - **slow**
- **Fast Gauss transform** to calculate matrix-vector products
  - "multipole" type hierarchic approximation
  - complexity $O(M + N)$
- **Low-rank approximation** to solve the linear equations
  - factorization of **G** by eigendecomposition precomputed
  - complexity $O(M)$

# Rigid 2D examples

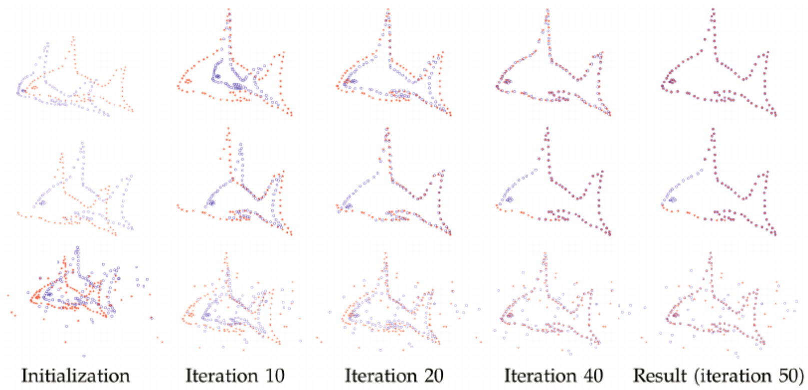


# Rigid 3D example

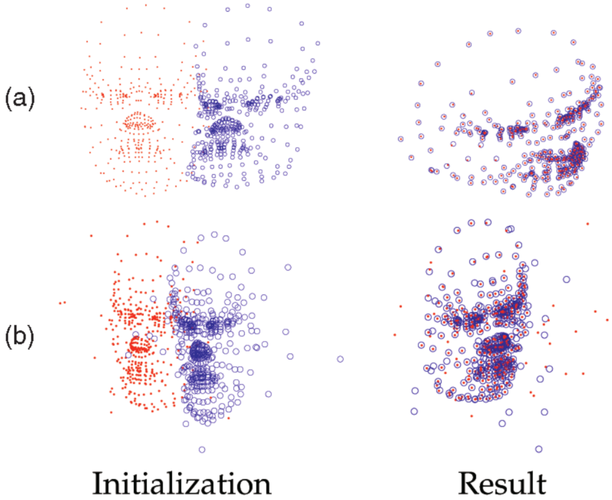


Initialization Iteration 10 Iteration 20 Iteration 30 Result (iteration 50)

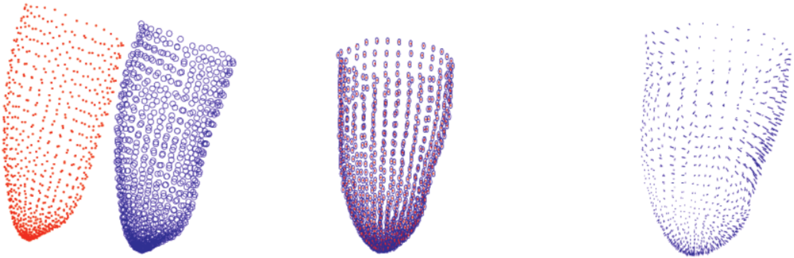
# Non-rigid 2D example



# Non-rigid 3D example



# 3D left ventricle matching



(a) (b) (c)

# CPD summary

- Relatively fast (seconds to minutes)
- Rigid, affine, non-linear transformation.
- Closed form rigid case
- Can be applied to 2D, 3D, $nD$
- Soft matching
- Robust to outliers and missing points (explicit modeling)
- Spatial coherence in the non-rigid case
- May fall to local minima