On the robust nonlinear curve fitting

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Motivation and Results

A large dimensional problem in a small dimensional space

- **Input vs feature space metric**: kernel method is a strong tool to deal with nonlinear problems by linear methods, but metric structure of input space is broken
  $\Rightarrow$ General framework to incorporate input space metric
- **Robustness**: L_p regularization ($p \leq 1$) is popular for the sparseness, but we focus more on L_p cost function for robustness
  $\Rightarrow$ Sparse property of the optimal solution
- **PCA vs MCA**: kernel PCA does not always give satisfiable results
  $\Rightarrow$ Comparative results (discussion) of kernel PCA and MCA

Acknowledgement

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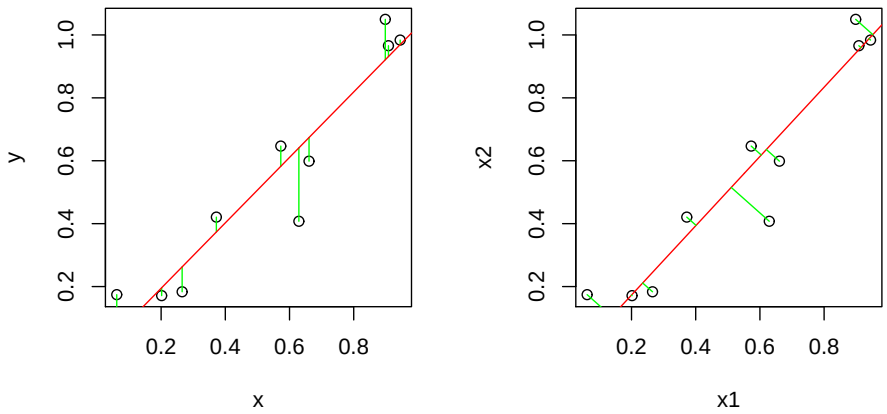
Fitting methods

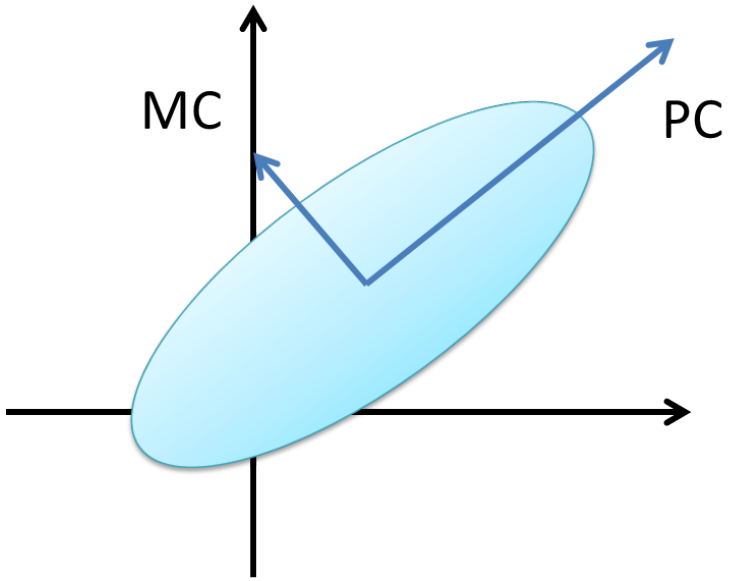
- **Purpose of fitting**: object recognition, denoising etc.
- There are (at least) two kinds of line/hypersurface fitting to sample points
  - **Regression** $y = f(\mathbf{x}) = \mathbf{a}^T\mathbf{x}$
    Distinctive treatment between y and $\mathbf{x}$
    Minimization of $E[(y - f(\mathbf{x}))^2]$
  - **Dimension reduction** $\mathbf{a}^T\mathbf{x} = 0$
    All components of $\mathbf{x}$ are treated equally
    Minimization of distance between points and line



Fitting by dimension reduction

- Minimization of distance between points and subspace (MCA)
- Equivalently, find the subspace that preserves variance of data points as much as possible (PCA)
- Equivalence of Principal Component Analysis (PCA) and Minor Component Analysis (MCA)
- Solution is obtained by solving eigenvalue problem

$$(X^T X)\mathbf{a} = \lambda \mathbf{a}$$



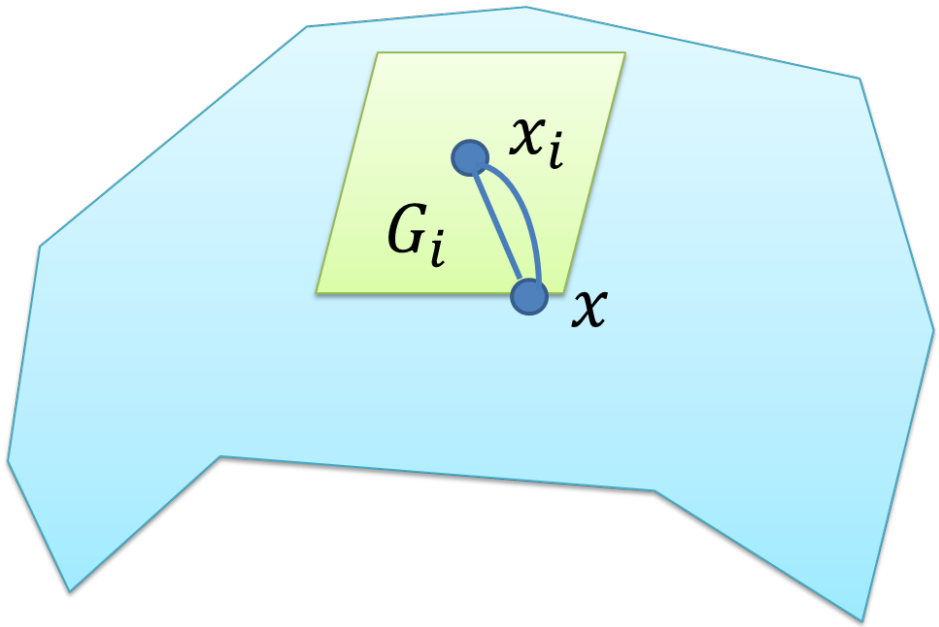
Extension to Riemannian space

In many applications, we need to consider non-Euclidean space

- Hypersphere (directional data, geology, economics; Fujiki+2007)
- Grassmann-Stiefel manifold (subspace data, independent component analysis; Nishimori+2005)
- Statistical manifold (statistics, optimization, control; Akaho2004)

Extension to Riemannian space

- Riemannian space with metric $G(\mathbf{x})$
- Extension to distance to the length of geodesic (hard to evaluate)
- Local approximation by the norm on the tangent space at $\mathbf{x}_i$
  $\|\mathbf{x} - \mathbf{x}_i\|^2_{G_i} = (\mathbf{x} - \mathbf{x}_i)^T G_i (\mathbf{x} - \mathbf{x}_i)$, $G_i = G(\mathbf{x}_i)$



- In spite of this approximation, dimension reduction problem cannot be solved by a simple eigenvalue problem.

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Quadratic curve fitting

- Quadratic curve fitting

$$a_0 + a_1 x_1 + a_2 x_2 + a_3 x_1^2 + a_4 x_1 x_2 + a_5 x_2^2 = 0$$

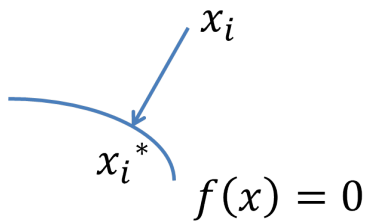
- Feature map reduces the nonlinear problem to linear problem
  $\mathbf{x} \mapsto \phi(\mathbf{x}) = (1, x_1, x_2, {x_1}^2, x_1 x_2, {x_2}^2)$
- Linear fitting on 6 dimensional feature space

Input space versus feature space

- Linear method on feature space minimizes the distance in feature space.
- However, the distance is not equal to the distance between points and the curve in the input space
- There are not many researches focusing on input space (Schölkopf 1999)

Locally linear approximation of function

- Projection from a point to a curve is difficult in general (local minimum/maximum, saddle)



- Linear approximation of $f(\mathbf{x}_i^*) = 0$ around $\mathbf{x}_i$ (Akaho1993)

$$0 = f(\mathbf{x}_i^*) \simeq f(\mathbf{x}_i) + \nabla f(\mathbf{x}_i)^T (\mathbf{x}_i^* - \mathbf{x}_i)$$

- The closest point $\mathbf{x}_i^*$ to $\mathbf{x}_i$ w.r.t. metric G_i, satisfying the constraint above is given by

$$\|\mathbf{x}_i^* - \mathbf{x}_i\|_{G_i}^2 = \frac{f(\mathbf{x}_i)^2}{\|\nabla f(\mathbf{x}_i)\|_{G_i^{-1}}^2}$$

Locally linear approximation of function

- Applying to $f(\mathbf{x}) = \mathbf{a}^T \phi(\mathbf{x})$ leads to the sum of input space distance

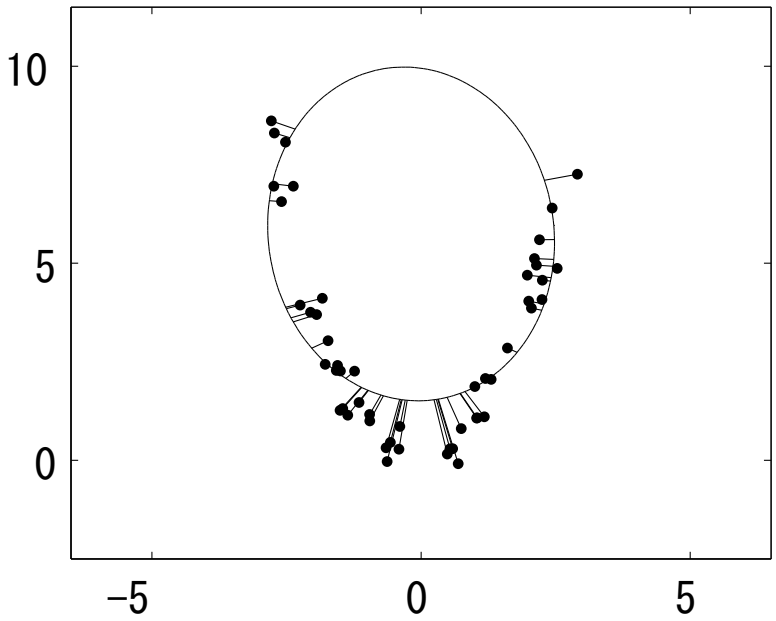
$$\sum_i \|\mathbf{x}_i^* - \mathbf{x}_i\|_{G_i}^2 = \sum_i \frac{\mathbf{a}^T \phi_i \phi_i^T \mathbf{a}}{\mathbf{a}^T \nabla \phi_i G_i^{-1} \nabla \phi_i^T \mathbf{a}}, \quad \phi_i = \phi(\mathbf{x}_i)$$

- Sum of ratio of quadratic forms
- Successive iteration method

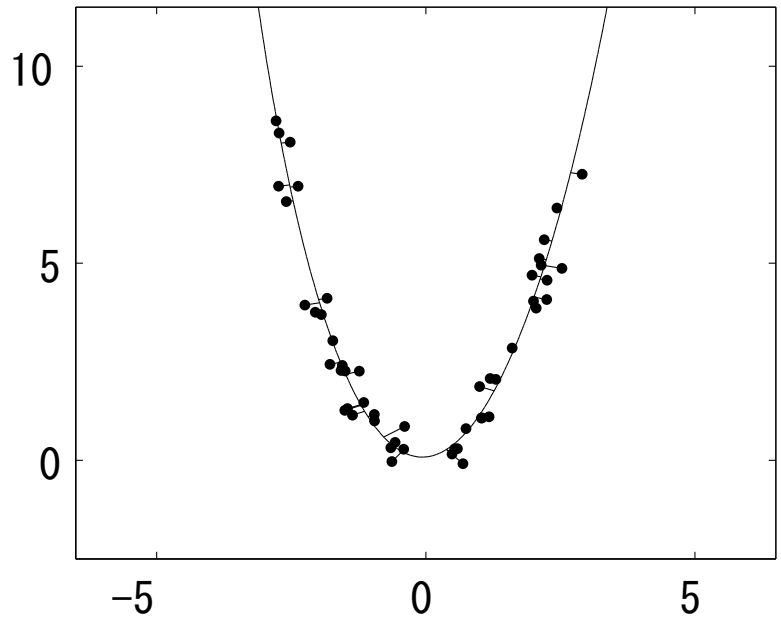
$$\mathbf{a}_{t+1} = \underset{\|\mathbf{a}\|=1}{\operatorname{argmin}} \mathbf{a}^T \left[\sum_i \frac{1}{w_i} \phi_i \phi_i^T \right] \mathbf{a}, \quad w_i = \mathbf{a}_t^T \nabla \phi_i G_i^{-1} \nabla \phi_i^T \mathbf{a}_t,$$

Example

$$u \sim \mathrm{u}[-2, 2], \quad x_1 = u + \epsilon_1, \quad x_2 = u^2 + \epsilon_2$$



Feature space



Input space

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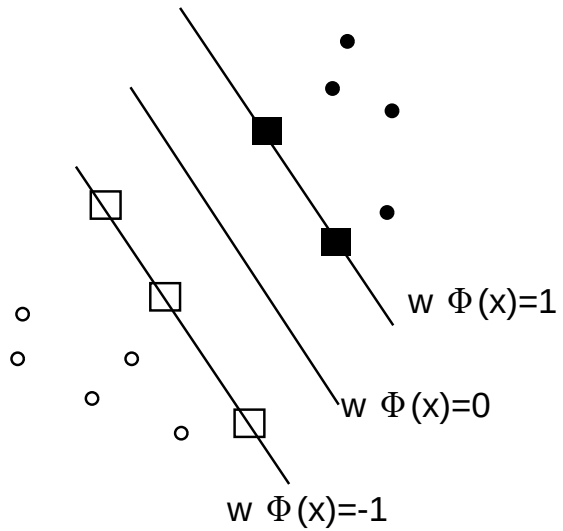
Toward higher dimensions

- Higher dimensional case (e.g. Reproducing Kernel Hilbert Space)
- First, we consider support vector machine (not curve fitting, but finds optimal separating hypersurface)
- Fitting problem is discussed later

Support vector machine

- SVM finds an optimal hyperplane that maximizes margin in the feature space
- Maximize the margin in the input space by the approximation of distance in the input space
- Approach: the same formulation as conventional SVM except introducing a linear approximation of distance (+ additional linear expansions; Akaho2004)

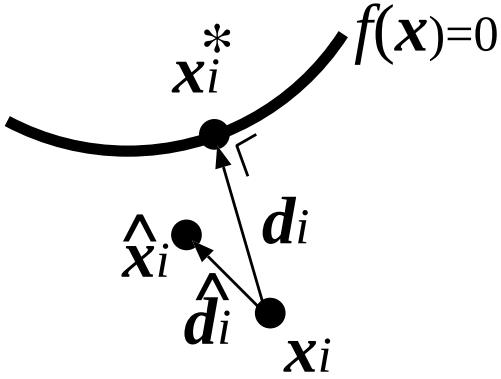


Approximation of distance

- Approximate the distance not around $\mathbf{x}_i$ but a better estimate $\hat{\mathbf{x}}_i$

$$\|\mathbf{d}_i\|^2_{G_i} = \frac{(\mathbf{a}^T\{\phi(\hat{\mathbf{x}}_i) - \nabla\phi(\hat{\mathbf{x}}_i)\hat{\mathbf{d}}_i\})^2}{\|\mathbf{a}^T\nabla\phi(\hat{\mathbf{x}}_i)\|^2_{G_i^{-1}}}$$

$$\mathbf{d}_i = \mathbf{x}_i^* - \mathbf{x}_i, \quad \hat{\mathbf{d}}_i = \hat{\mathbf{x}}_i - \mathbf{x}_i$$



- $\hat{\mathbf{x}}_i$ is initialized by $\mathbf{x}_i$ and it can be iteratively improved (discussed later)

Margin constraint

- Separating hyperplane is invariant under scalar transformation of $\mathbf{a}$, so we assume

$$\min_i \|\mathbf{d}_i\|_{G_i}^2 = \frac{1}{\|\mathbf{a}\|^2}$$

- Then maximizing margin is equivalent to minimizing $\|\mathbf{a}\|^2$ (quadratic regularization) under the above constraints with sign

$$y_i \frac{\mathbf{a}^T\{\phi(\hat{\mathbf{x}}_i) - \nabla\phi(\hat{\mathbf{x}}_i)\hat{\mathbf{d}}_i\})}{\|\mathbf{a}^T\nabla\phi(\hat{\mathbf{x}}_i)\|_{G_i^{-1}}^2} \geq \frac{1}{\|\mathbf{a}\|}$$

Linearization of constraints

- Suppose an approximate solution $\hat{\mathbf{a}}$ is given, we approximate the constraint by linear inequality of $\mathbf{a}$

$$\mathbf{a}^T[y_i\{\phi(\hat{\mathbf{x}}_i) - \nabla\phi(\hat{\mathbf{x}}_i)\hat{\mathbf{d}}_i\} - \hat{\boldsymbol{\eta}}_i] \geq \hat{g}_i$$

  where $\hat{g}_i$: scalar function, $\hat{\boldsymbol{\eta}}_i$: linear function of $\nabla\phi(\hat{\mathbf{x}}_i)$ and $\hat{\mathbf{a}}$

- Quadratic optimization with linear constraint leads to

$$L(\mathbf{a}) = \mathbf{a}^T\mathbf{a} - \sum_{i=1}^{n} \alpha_i \left(\mathbf{a}^T[y_i\{\phi(\hat{\mathbf{x}}_i) - \nabla\phi(\hat{\mathbf{x}}_i)\hat{\mathbf{d}}_i\} - \hat{\boldsymbol{\eta}}_i] - \hat{g}_i\right)$$

  where α_i is a Lagrange multiplier

Support Vectors

- Differentiating $L(\mathbf{a})$ by $\mathbf{a}$, we have

$$\mathbf{a} = \sum_{i=1}^{n} \alpha_i [y_i \{\phi(\hat{\mathbf{x}}_i) - \nabla\phi(\hat{\mathbf{x}}_i)\hat{\mathbf{d}}_i\} - \hat{\boldsymbol{\eta}}_i]$$

- Sparsity (some α_i are exactly 0 as in SVM)
- Classification function $f(\mathbf{x}) = \mathbf{a}^T\phi(\mathbf{x})$:
  if we assume $\hat{\mathbf{a}}$ is a linear function of $\phi(\hat{\mathbf{x}}_i)$ and $\nabla\phi(\hat{\mathbf{x}}_i)$,

$$f(\mathbf{x}) = \sum_i \{a_i \phi(\hat{\mathbf{x}}_i)^T \phi(\mathbf{x}) + b_i \nabla\phi(\hat{\mathbf{x}}_i)^T \phi(\mathbf{x})\}$$

(Since $\hat{\boldsymbol{\eta}}_i$ is a linear function of $\hat{\mathbf{a}}$ and $\phi(\hat{\mathbf{x}}_i)$)

Kernelization

- Reproducing kernel Hilbert space
- Kernel function (strictly it should be written as an inner product)

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$$

- Derivative of kernel function

$$\nabla_{\mathbf{x}} k(\mathbf{x}, \mathbf{x}') = \nabla \phi(\mathbf{x})^T \phi(\mathbf{x}'),$$

$$\nabla_{\mathbf{x}} \nabla_{\mathbf{x}'} k(\mathbf{x}, \mathbf{x}') = \nabla \phi(\mathbf{x})^T \nabla \phi(\mathbf{x}')$$

Kernel trick

- Kernel trick enables us to choose positive semidefinite function as a kernel function instead of taking inner product in the feature space
- Example (Gaussian kernel)
  - $k(\mathbf{x}, \mathbf{x}') = \exp(-\beta\|\mathbf{x} - \mathbf{x}'\|^2)$
  - $\nabla_{\mathbf{x}} k(\mathbf{x}, \mathbf{x}') = -2\beta k(\mathbf{x}, \mathbf{x}')(\mathbf{x} - \mathbf{x}')$,
  - $\nabla_{\mathbf{x}} \nabla_{\mathbf{x}'} k(\mathbf{x}, \mathbf{x}') = 2\beta k(\mathbf{x}, \mathbf{x}')(I - 2\beta(\mathbf{x} - \mathbf{x}')(\mathbf{x} - \mathbf{x}')^T)$,
- Kernel version of classification function

$$f(\mathbf{x}) = \sum_i \{a_i k(\hat{\mathbf{x}}_i, \mathbf{x}) + b_i \nabla k(\hat{\mathbf{x}}_i, \mathbf{x})\}$$

Estimation of $\hat{x}_i$

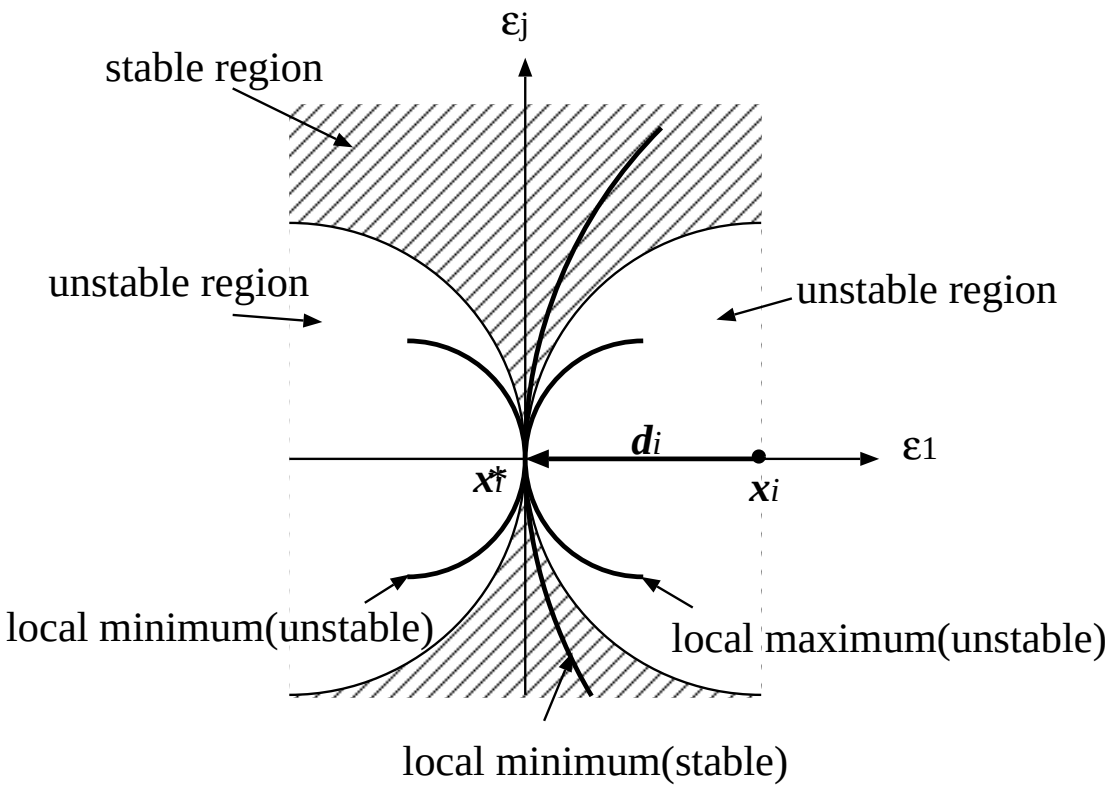
- $\hat{\mathbf{x}}_i$ can be improved for a fixed parameter of curve $\hat{\mathbf{a}}$

$$\mathbf{x}_i^{[l+1]} = h(\mathbf{x}_i^{[l]}, \hat{\mathbf{a}}, \mathbf{x}_i, G_i)$$

- It may converge to a local minimum, a local maximum, or a saddle point. How about the convergence property?
- **Property of the iterative solution**: Let $\mathbf{x}_i^*$ be an equilibrium state of the iteration step, it is a critical point of the projection point (a local minimum/maximum, or saddle point). If it is a local maximum or saddle, the algorithm is always unstable

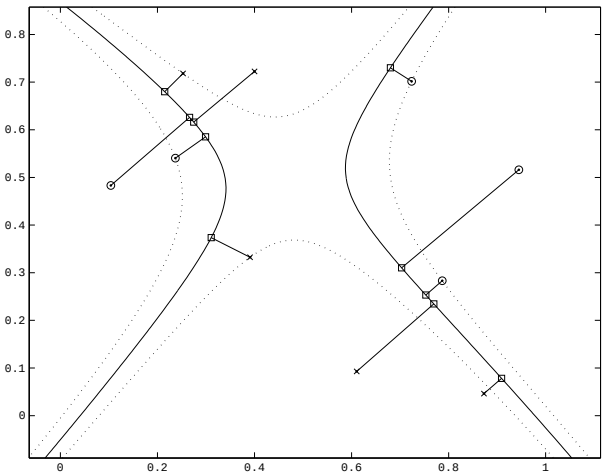
Estimation of $\hat{x}_i$

For a local minimum, the curvature of the hypersurface determines the stability (we can slow down the iteration step to avoid the instability)

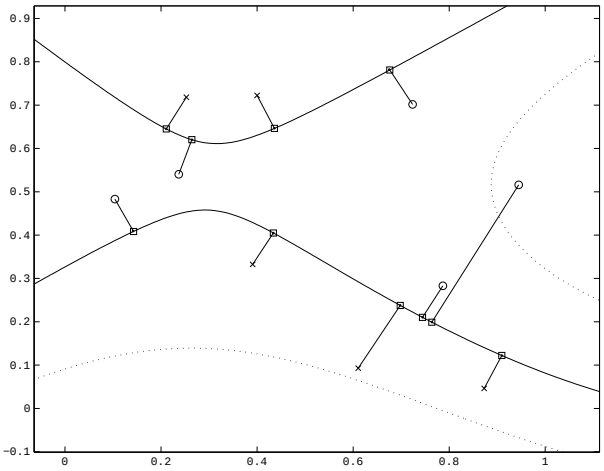


Example

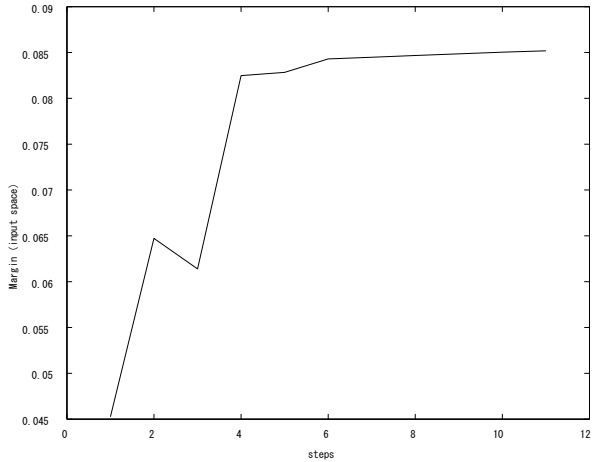
- Through experiments for synthetic and some benchmark datasets, we showed that the input space margin and generalization performance increased by a proposed method



Original



Input space



Margin

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Robustness and sparseness

- Typical optimization formulation for fitting

$$E = \sum_i \mathrm{Cost}(\mathbf{x}_i, f) + \lambda \mathrm{Reg}(f)$$

- Regularization: we don't discuss in detail here
  SVM: L_2, Lasso: L_1 (sparse prior)
- Cost:
  -SVM: Hinge loss of $[yf(\mathbf{x}) - 1]_+$
  -Ordinary regression: Quadratic loss $(y - f(\mathbf{x}))^2$
  -Fitting by dimension reduction: Quadratic (vertical) distance
  -Here: p-th power (vertical) distance (robust + sparseness)

p-th power deviation

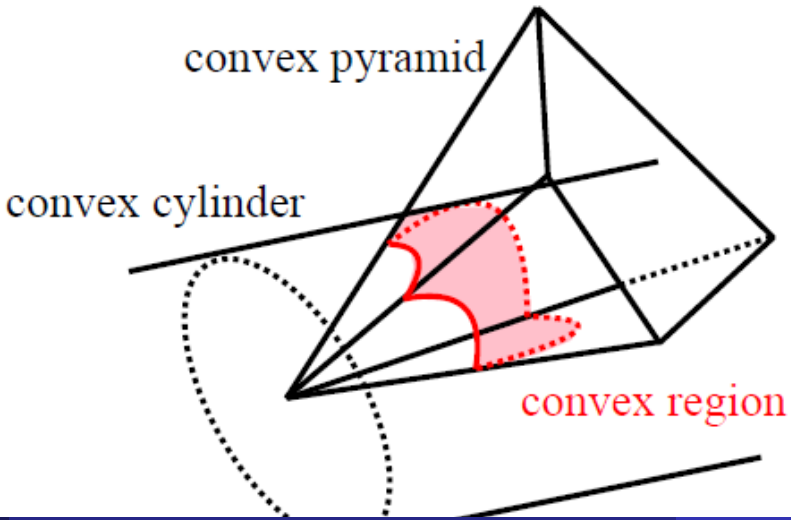
- Euclidean distance from a d-dim point $\mathbf{x}_i$ to a hyperplane $\mathbf{a}^T\mathbf{x} + a_0 = 0, \|\mathbf{a}\| = 1$ is given by $|\mathbf{a}^T\mathbf{x}_i + a_0|$
- Minimizing the mean p-th power of the Euclidean distance

$$R_p(\mathbf{a}) = \sum_{i=1}^{n} w_i |\mathbf{a}^T\mathbf{x}_i + a_0|^p$$

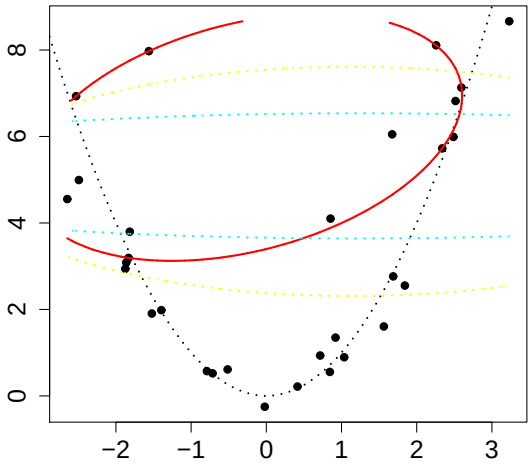
- R_1 norm (Ding2006)
- R_0 is meaningless (the same cost values)
- We can prove L_p $0 < p \leq 1$ case is completely sparse (the optimal hyperplane passes through d points)

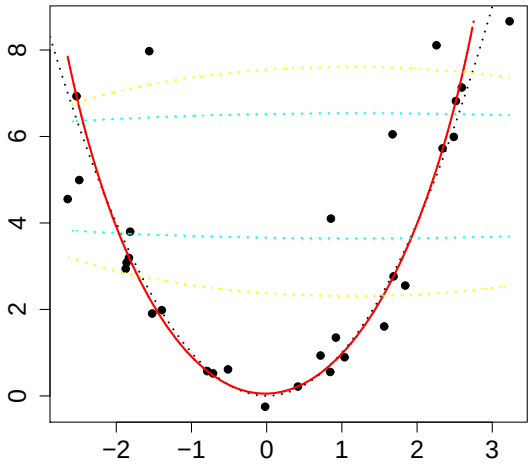
Proof sketch

- The parameter $(\mathbf{a}^T, a_0)$ is on a cylinder $Q = S^d \times R$: convex in R^{d+1} against the origin
- Parameter space is devided by n hyperplanes $\mathbf{a}^T\mathbf{x}_i + a_0 = 0$, each P is convex in R^{d+1}. $\Rightarrow P \cap Q$ is convex against the origin
- The (weighted) p-th deviation takes concave contour against origin
- The minimum of the objective function is obtained in the boundary of $P \cap Q$
- The procedure is performed recursively, and the (local) minimum is obtained at one of the vertex of P



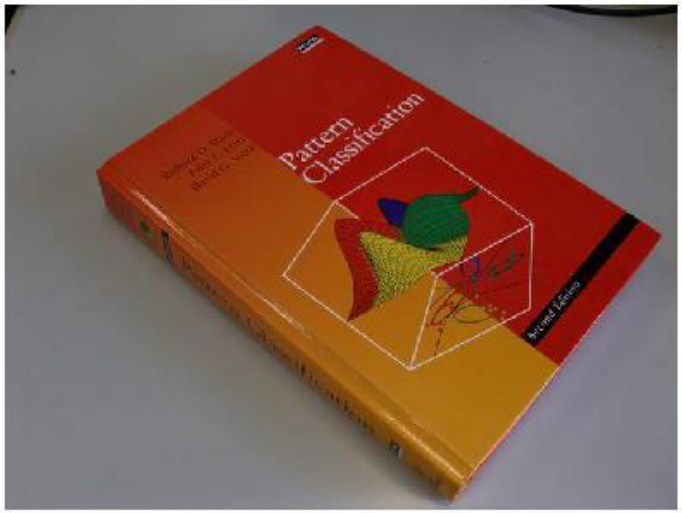
Example



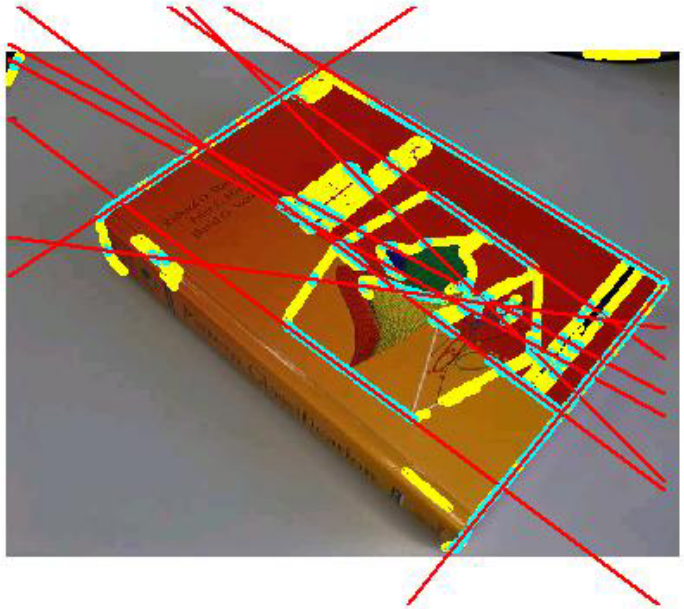


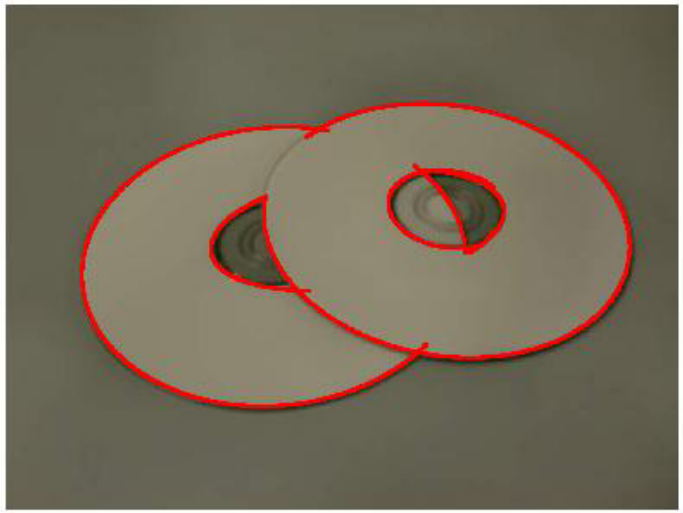
Feature space ($p = 0.5$) Input space ($p = 0.5$)
(Yellow (Feature space $p = 2$) and Blue (Input space $p = 2$))

Example



Example





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Curve fitting in RKHS

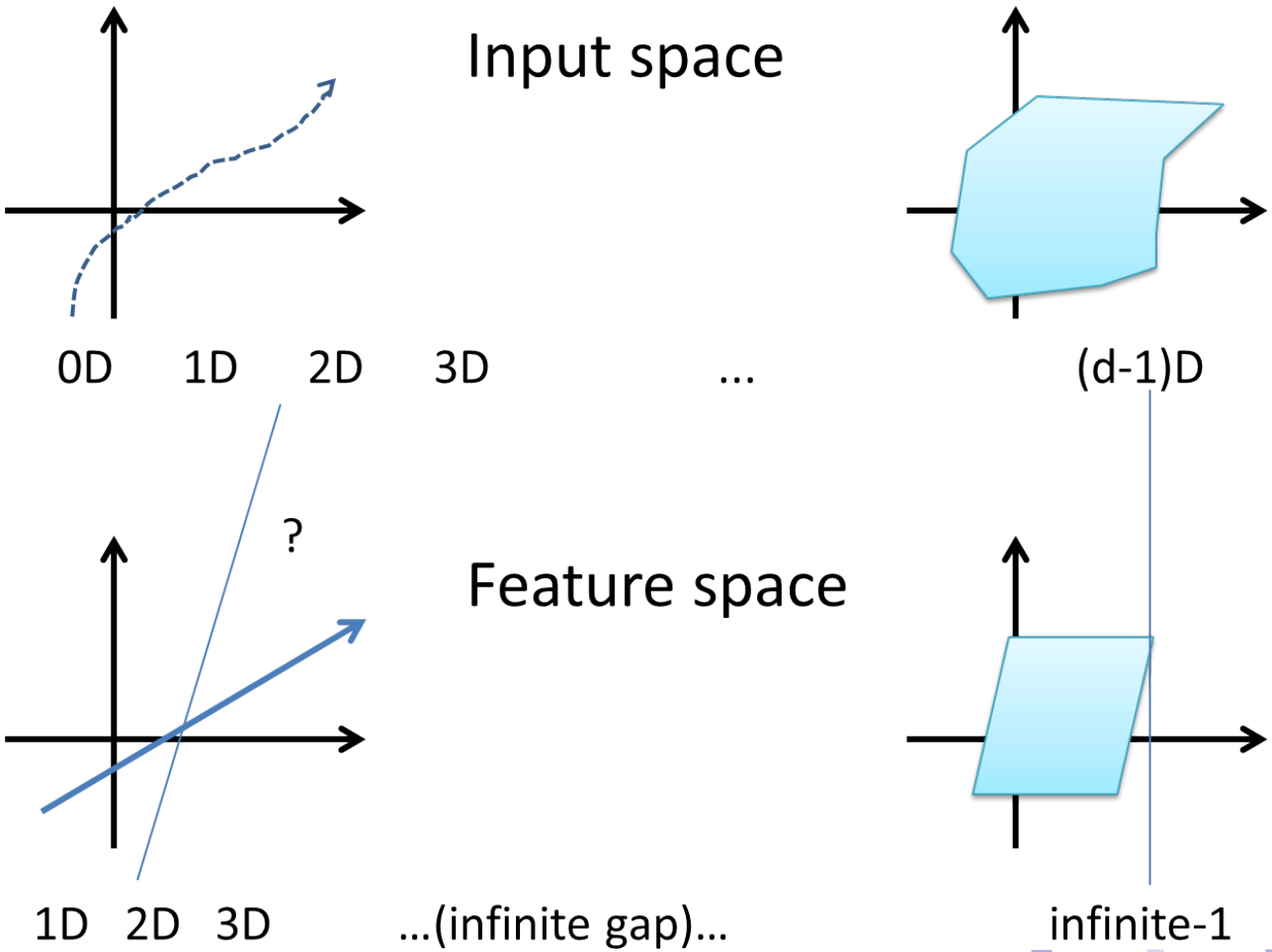
- We want to extend the curve fitting in high dimensional space
- PCA vs MCA (in low dimensional case, it is almost equivalent)
- In infinite dimensional case, the difference taking higher eigenvalues and discarding lower eigenvalues is large
- Note: finding a dimension reduction map $u = f(x)$ and finding a low dimensional structure $x' = g(x)$ in the input space are slightly different

Minor component analysis

- In the first part of my talk, we considered the hyperplane $\mathbf{a}^T \phi(\mathbf{x}) = 0$ which is obtained by MCA
- MCA is attractive because to find the optimal hyperplane was somewhat reasonable in SVM
- But in MCA case, it is hard because of too much degree of freedom

PCA vs MCA

- The image of input space in feature space is very sparse
- PCA (small number of projection axes)
- MCA (small number of noise reduction axes)



Two kinds of regularization

- Tikhonov (SVM)

$$\min_f \sum_i \mathrm{Cost}(f(\mathbf{x}_i)) + \lambda\Omega(\|f\|)$$

  $f \in$ RKHS, Ω is a nondecreasing function

- Ivanov-like (PCA, MCA) not precisely Ivanov

$$\min_f \sum_i \mathrm{Cost}(f(\mathbf{x}_i)) \quad \text{s.t.} \quad \|f\| = \text{const}$$

Representer theorem

- Representer theorem is a key theorem for RKHS, which reduces the dimensionality from infinite to finite
- **Representer theorem 1**: As for Tikhonov regularization

$$\min_f \sum_i \mathrm{Cost}(f(\mathbf{x}_i)) + \lambda\Omega(\|f\|),$$

For any Cost function, the optimal f is in the form

$$f_{opt}(\mathbf{x}) = \sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x})$$

Ivanov-like

- **Representer theorem 2**: As for Ivanov-like regularization

$$\min_f \sum_i \mathrm{Cost}(f(\mathbf{x}_i)) \quad \text{s.t.} \quad \|f\| = \text{const}$$

If the Cost function satisfies decreasing property ($Cost(c_1 f(\mathbf{x})) \leq Cost(c_2 f(\mathbf{x}))$ when $c_1 \geq c_2 > 0$), the optimal f is in the form

$$f_{opt}(\mathbf{x}) = \sum_i \alpha_i k(\mathbf{x}_i, \mathbf{x})$$

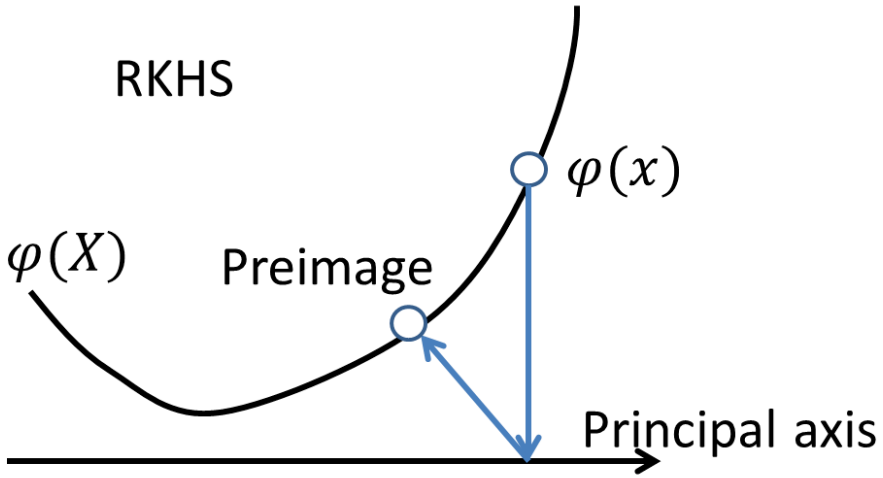
- PCA (minus of variance of $f(\mathbf{x}_i)$) satisfies, but MCA (variance of $f(\mathbf{x}_i)$) does not! Even data out of samples can be good for MCA.

Approach from PCA

- Kernel PCA does not work as one would expect (cf. manifold learning)
- For noise reduction, we need to solve "preimage problem" that is difficult to solve
- Even if preimage is found, it is not always what we want (non-smooth, more dimension is needed)
- The structures of projection and preimage are different in nonlinear case

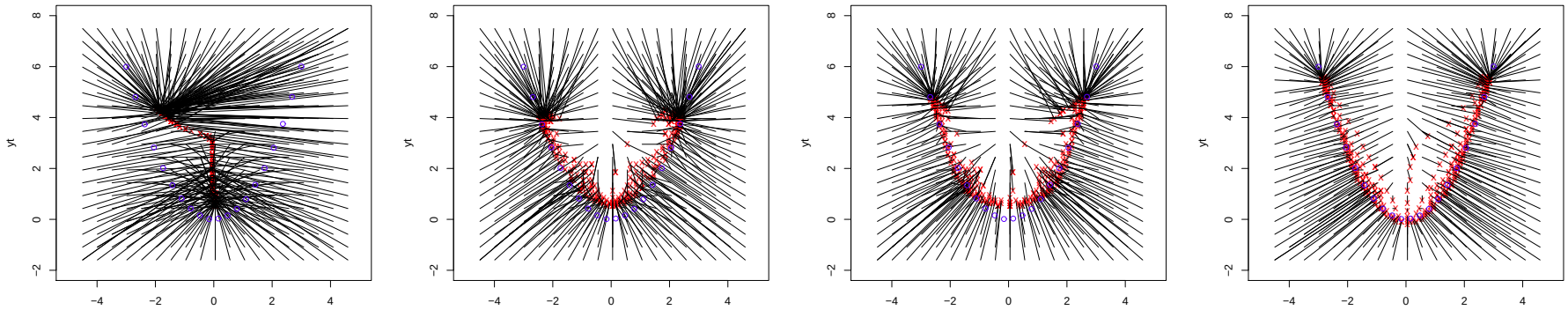
Preimage

Finding a dimension reduction map $u = f(x)$ and finding a low dimensional structure $x' = g(x)$ in the input space are slightly different in nonlinear case



Example

Preimage is somewhat unstable and not smooth

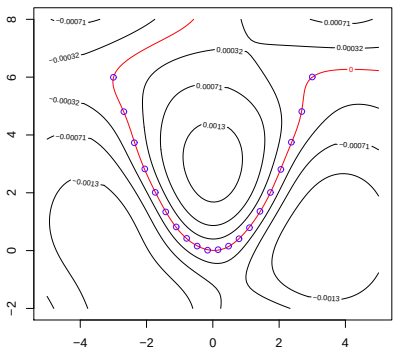
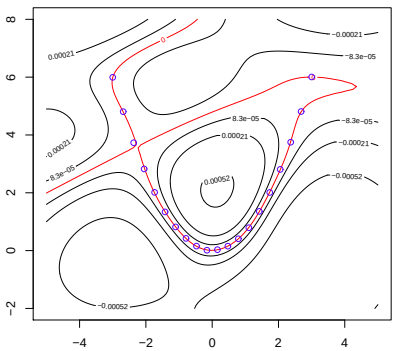
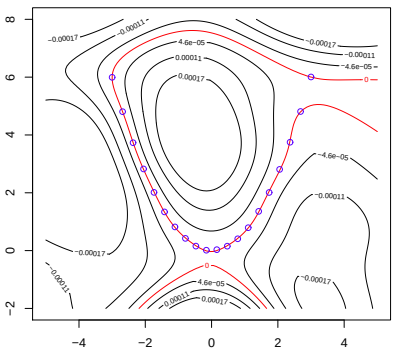
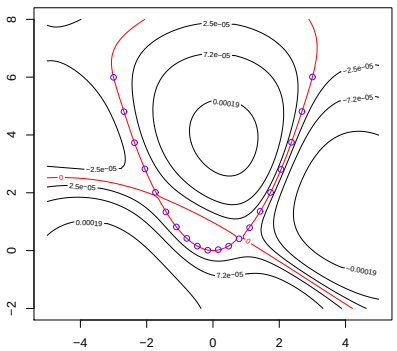


Approach from MCA

- Kernel MCA achieves smoother curve/surface
- Too many freedom (even in the sample space)

Example

MCA gives too many good curves! (their linear combination as well; Fujiki+2013)
Further out of sample points will increase the freedom
Does sparsity help to choose a good curve? $\rightarrow$ open

Concluding remarks

- The method to incorporate input space metric is proposed
- Finding the projection point to hypersurface is more stable than finding the preimage
- L_p cost function is effective when many outliers exist
- MCA has a potential to give a good curve fitting, but choosing a good curve obtaining good generalization performance is not established