Principal Component Analysis: Linear and Nonlinear Methods

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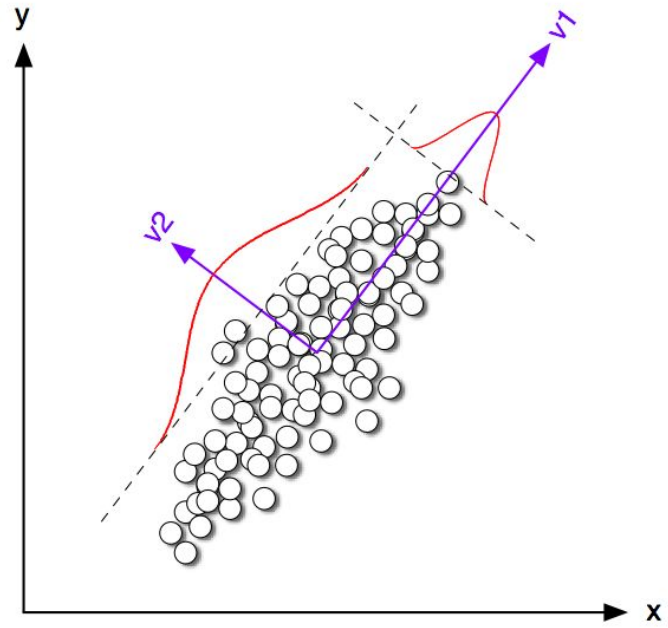
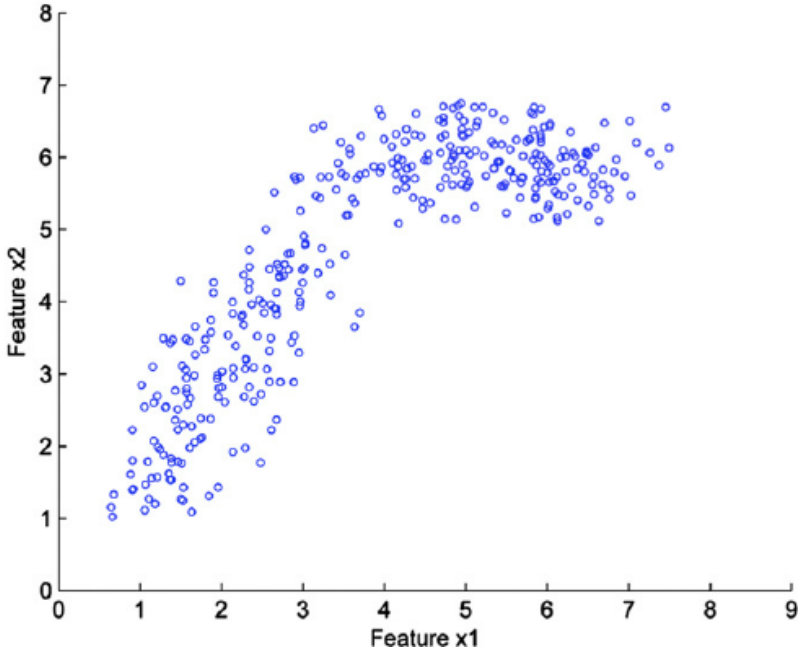
Principal Component Analysis

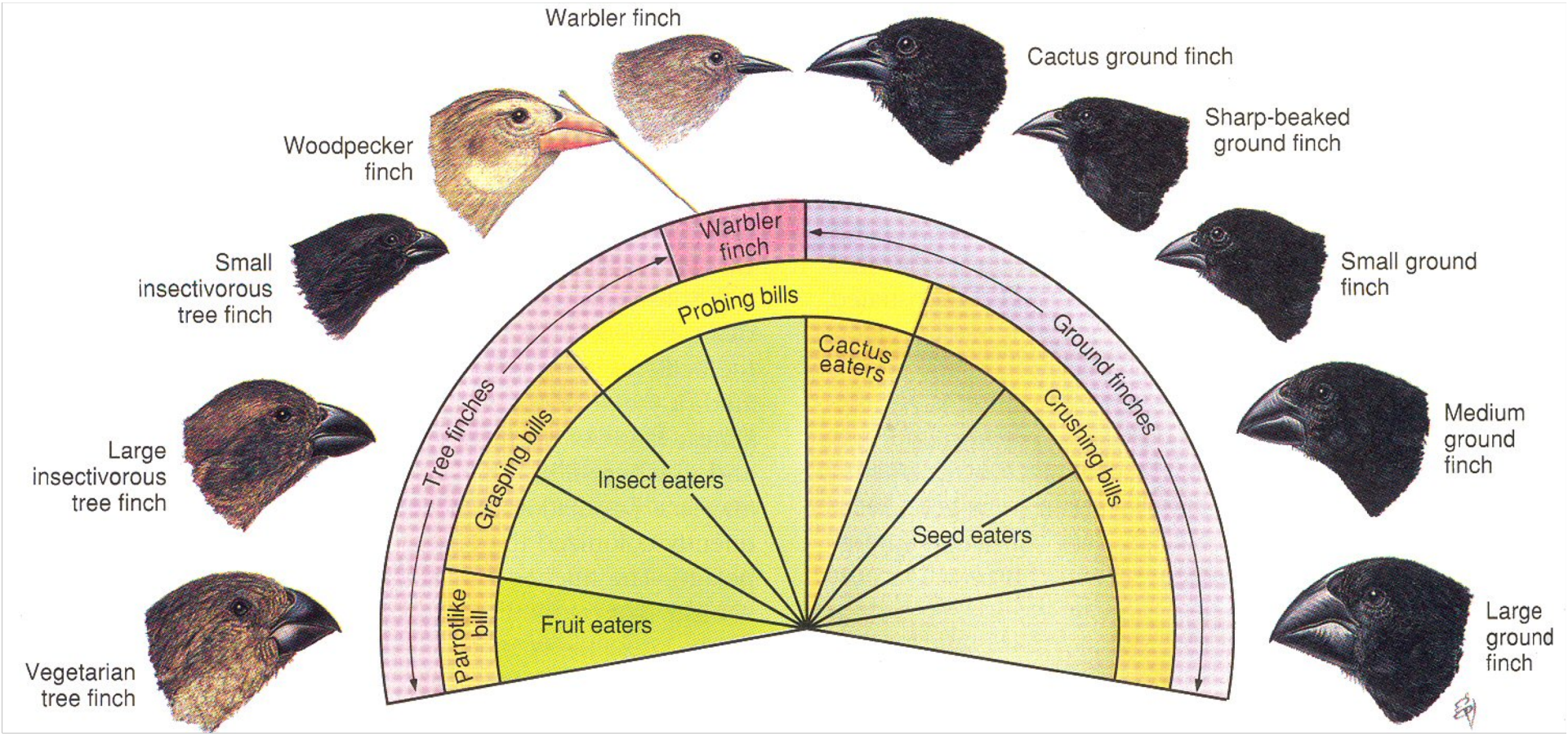
- Statistical model of the data
  - Finding the mean of the data sample
  - Finding modes of variation in data sample
- Very closely related to fitting a multivariate Gaussian model to the data





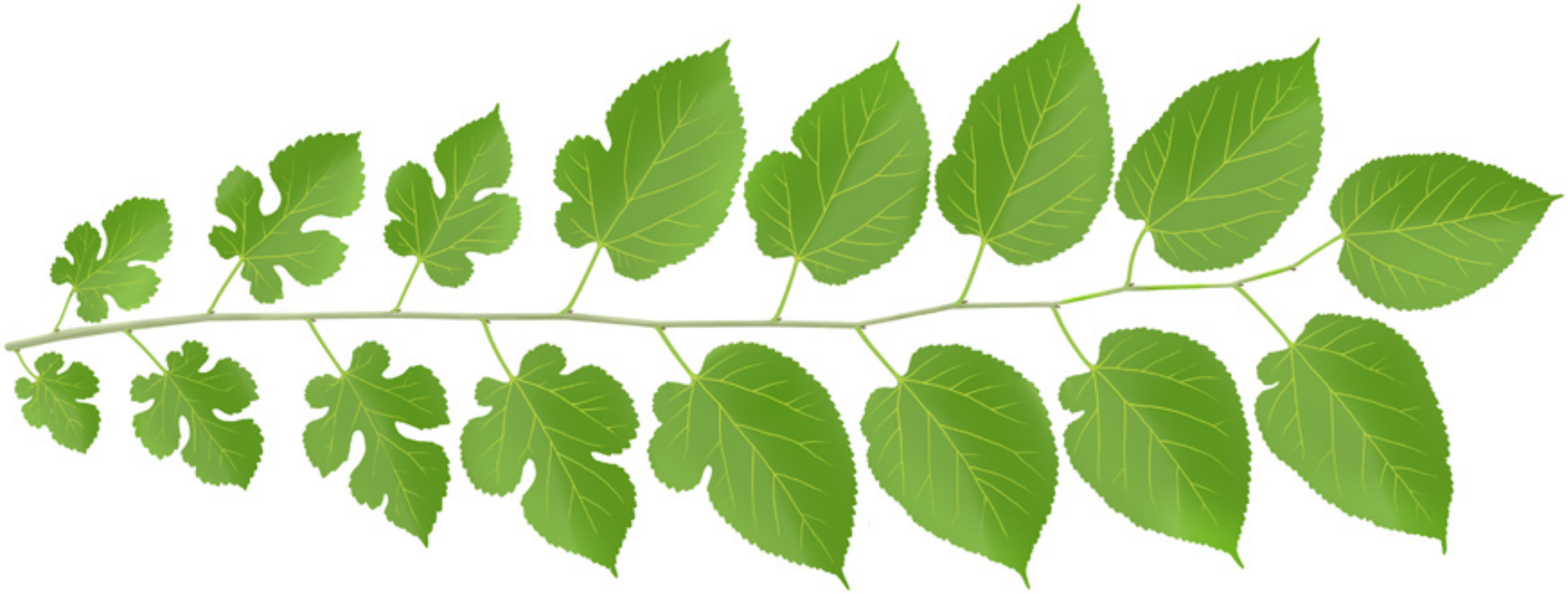
Principal Component Analysis

- Darwin's finches
  - Variation of beak's shape and size



Principal Component Analysis

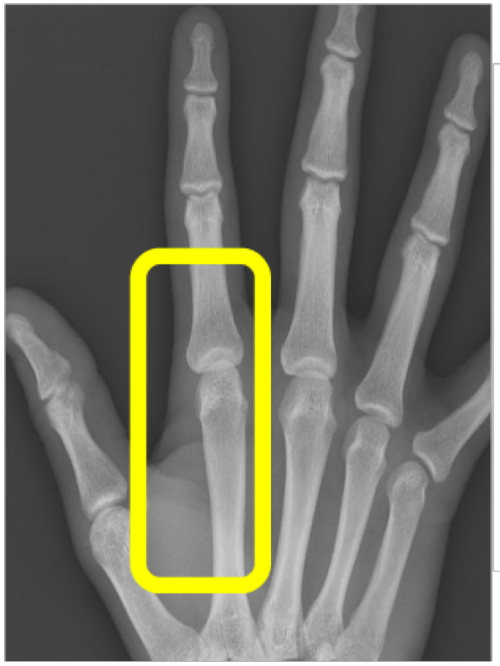
- White mulberry leaves
  - Simpler leaves reflect maturity



http://www.washingtonpost.com/wp-srv/special/metro/urban-jungle/pages/120724.html

Principal Component Analysis

- Human wrist bone



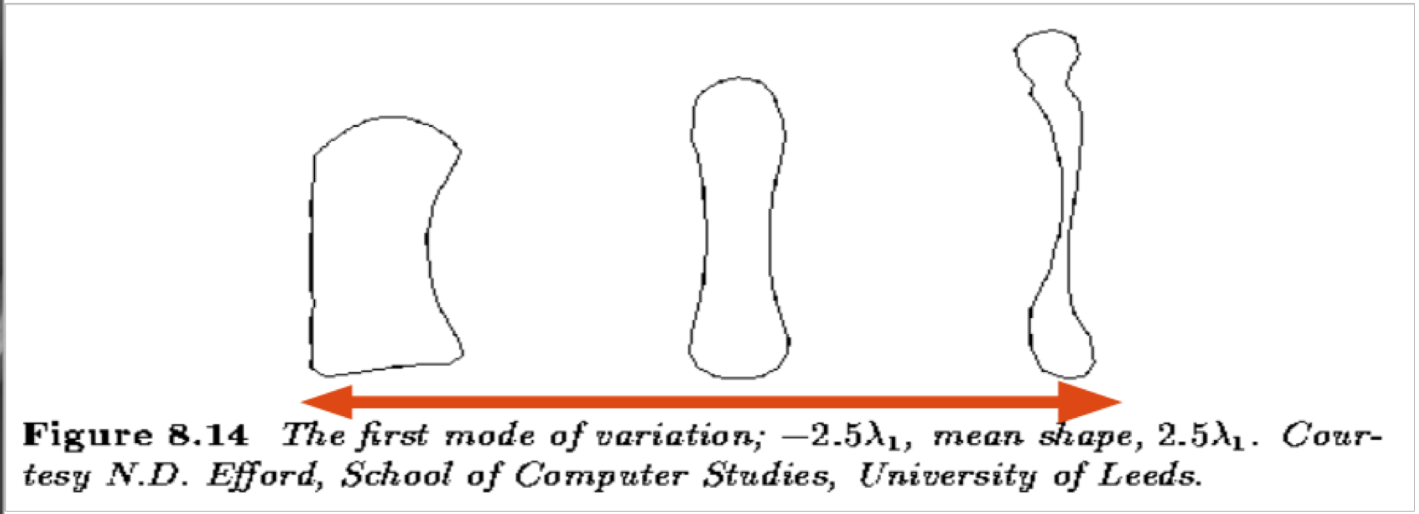
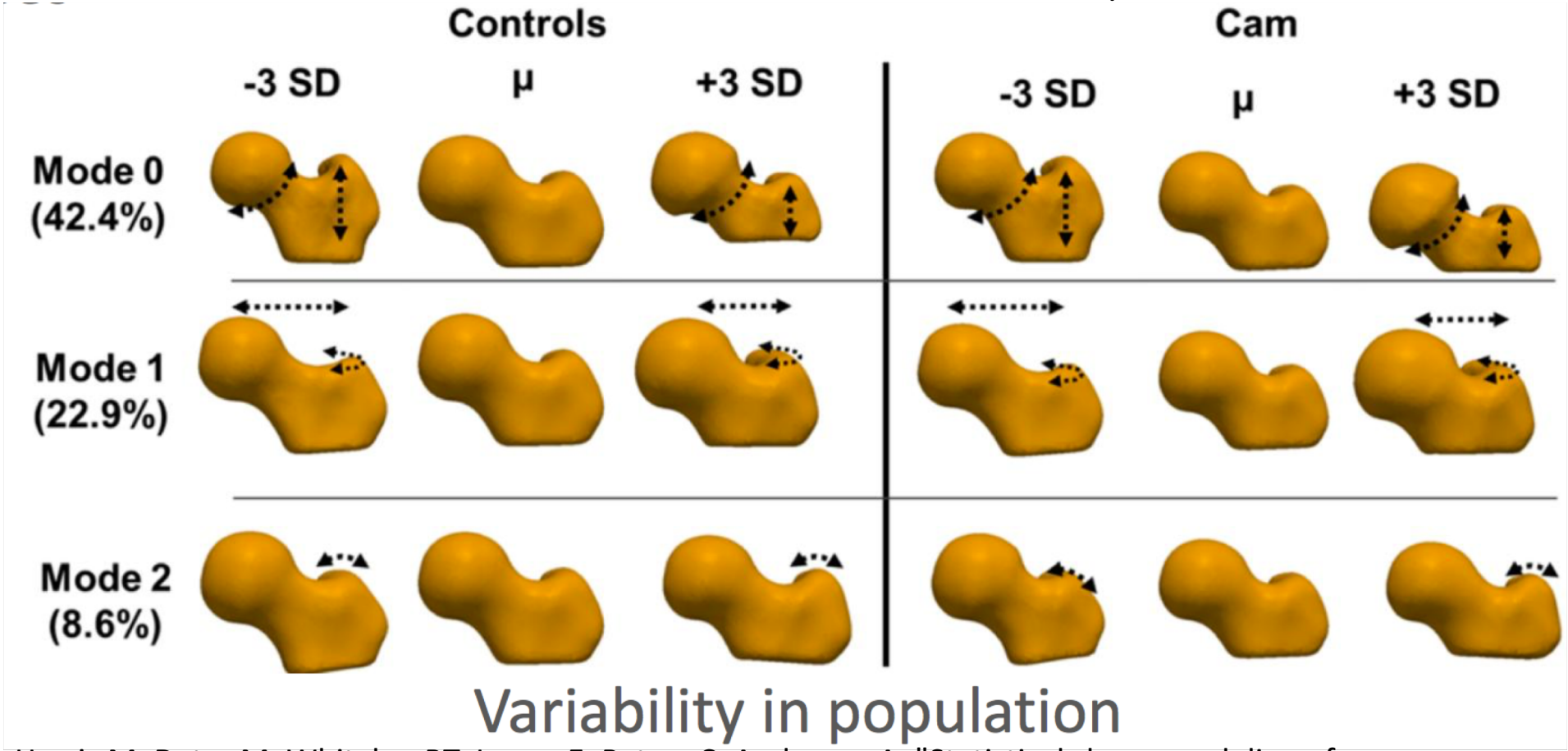


Figure 8.14 *The first mode of variation; $-2.5\lambda_1$, mean shape, $2.5\lambda_1$. Courtesy N.D. Efford, School of Computer Studies, University of Leeds.*

Principal Component Analysis

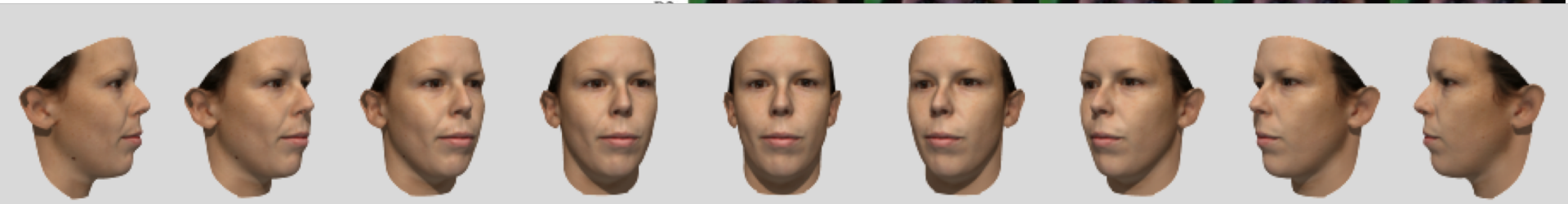
- Human hip bone
  - Modes of variation in normal cases, diseased cases



Harris M, Datar M, Whitaker RT, Jurrus E, Peters C, Anderson A. "Statistical shape modeling of cam femoroacetabular impingement." *Journal of Orthopaedic Research* 31, no. 10 (2013): 1620-1626.

Principal Component Analysis

- Face recognition
  - Variability in appearance



Pose Variations (-70, -50, -30, -15, 0, 15, 30, 50, 70 degree rotation around Y-axis)

Illumination Variations (0, 30, 50 degree rotation around Y-axis)

Multivariate Gaussian

- Generalizes a univariate Gaussian probability density function (PDF)
  - Standard normal density function = 1D Gaussian with mean 0, standard deviation 1
- Consider a vector random variable (RV) $X := [X_1, X_2, \ldots, X_D]^T$

Multivariate Gaussian

- **Definition**
  - The random variable (RV) $X := [X_1, X_2, \ldots, X_D]^T$ has a multivariate (jointly) Gaussian PDF if there exists a finite set of independent and identically distributed (i.i.d.) univariate standard-normal RVs $W_1, \ldots, W_N$ (with $D <= N$) such that each X_d can be expressed as

$$X_d = \mu_d + \sum_n A_{dn} W_n \text{ (i.e., } X = AW + \mu)$$

Multivariate Gaussian

- Example 1: **Zero-Mean Isotropic Gaussian**
  - Consider independent standard-normal RVs $W_1,\ldots,W_D$ with $A = I_{D\times D}$ and $\mu = 0$
  - Then, $X = AW + \mu = W$
  - Then, the Gaussian PDF is:

$$p(w) = \prod_d p(w_d) = \frac{1}{(2\pi)^{d/2}} \exp(-0.5 w^T w)$$

Multivariate Gaussian

- Transformation of random variables
  - Univariate case: W is 1-dimensional with PDF P(W)
    - Consider a function g(.) such that X := g(W)
    - Then, PDF of X is:

$$p(g^{-1}(x)) \left| \frac{d}{dx} g^{-1}(x) \right|$$

  - Multivariate case: W is D-dimensional with PDF P(W)
    - Consider the transformation X := A W
    - Then, the PDF of X is:

$$q(X) = p(A^{-1}X) \frac{1}{\det(A)} = \frac{1}{(2\pi)^{d/2} \det(A)} \exp(-0.5 X^T (A^{-1})^T A^{-1} X)$$

    - If C := AA^T (where C has a special name), then $q(X) = \frac{1}{(2\pi)^{d/2} |C|^{0.5}} \exp(-0.5 X^T C^{-1} X)$

Multivariate Gaussian

- Example 2: **Zero-Mean Anisotropic Gaussian**
  - Consider the case where
    $\mu = 0$ and A is a square non-singular matrix
  - Then, the Gaussian PDF is:

$$q(X) = \frac{1}{(2\pi)^{d/2}|C|^{0.5}} \exp(-0.5X^T C^{-1} X)$$

  - Property
    - When X = AW,
      E[X] = E[AW] = A E[W] = 0

Multivariate Gaussian

- Example 3: **Anisotropic Gaussian**
  - When X = AW and Y = X + μ = **AW + μ**
    - E[Y] = E[AW + μ] = A E[W] + μ = μ
    - And the PDF is:

$$p(y) = \frac{1}{(2\pi)^{d/2}|C|^{0.5}} \exp(-0.5(y-\mu)^T C^{-1}(y-\mu))$$

Multivariate Gaussian

- For any multivariate RV X
  - Covariance C := E [$(X-\mu)(X-\mu)^T$]
  - Thus, C_{ij} = E [$(X_i-\mu_i)(X_j-\mu_j)^T$] = Cov (X_i, X_j)
- Property: Cov (W) = E [WW^T] = I
  - Cov (W_i, W_i) = 1 (standard normal PDF)
  - Cov (W_i, $W_{j\sim i}$) = 0 (independence)
- For a multivariate Gaussian RV X = AW + μ
  - Property: Cov (X) = Cov (AW + μ)
    = E [$(AW)(AW)^T$] = A^T E[WW^T] A = A^T A

$$p(y) = \frac{1}{(2\pi)^{d/2}|C|^{0.5}} \exp(-0.5(y-\mu)^T C^{-1}(y-\mu))$$

Multivariate Gaussian

- **Covariance matrix**
  - Property: C is **symmetric**
    - $C_{ij} = Cov(X_i, X_j) = Cov(X_j, X_i) = C_{ji}$
  - Property: C is **positive semi-definite** (PSD)
    - For any non-zero vector 'a',
      $E[a^T (X - E[X])(X - E[X])^T a] = E[(f(X))^T f(X)] >= 0$
      = variance of scalar RV $f(X) := (X - E[X])^T a$

Multivariate Gaussian

- **Eigen Decomposition**
  - Every square matrix M
    has an eigen-decomposition $M = Q \Lambda Q^{-1}$
    where
    Q is an invertible matrix
    Λ is a diagonal matrix
  - Every square real symmetric matrix M
    (like the covariance matrix C)
    has an eigen-decomposition $M = Q \Lambda Q^{T}$
    where
    Q is an orthogonal matrix
    Λ is a diagonal matrix

Multivariate Gaussian

- Eigen Decomposition
  - Every square real symmetric PSD matrix M
    (like the covariance matrix C)
    has an eigen-decomposition $M = Q \Lambda Q^T$
    where
    Q is an orthogonal matrix
    Λ is a diagonal matrix with nonnegative entries

Multivariate Gaussian

- **Contours of the multivariate Gaussian PDF**
  - Property: If X is multivariate Gaussian in 2D with a diagonal (invertible) covariance C, then iso-probability contours of P(X) are ellipses whose axes are aligned with the cardinal axes
  - Proof:
    - Let C be symmetric positive definite (SPD)
    - C^{-1} is also SPD
      - C has a Cholesky decomposition $C = MM^T$, where M is upper triangular with positive diagonal entries
      - $C^{-1} = (M^T)^{-1} (M)^{-1} = NN^T \rightarrow$ SPD
    - A contour $\{x: P(x) = \alpha\}$
      $= \{x: (x-\mu)^T C^{-1} (x-\mu) = \beta\}$ where $\beta>0$ because C^{-1} is SPD
      $= \{x: \Sigma_d (x_d - \mu_d)^2 / (\beta\sigma_d^2) = 1\}$ that is an ellipse

Multivariate Gaussian

- **Mahalanobis Distance**
  - $(x-\mu)^T C^{-1} (x-\mu)$
  - Multidimensional generalization of Euclidean distance from mean μ
    - Rescales units along each dimension, based on the variance of the data along that dimension
  - Iso-probability contour of a Gaussian is the locus of points with the same Mahalanobis distance
  - Theorem:
    Mahalanobis distance is a true distance metric
    - Satisfies positivity, symmetry, triangular inequality

Multivariate Gaussian

- **Scaling and Rotating the coordinate frame**
  - Let X := SW
    - S = diagonal matrix that rescales units along each coordinate axis
    - Covariance matrix $C = SS^T = S^2$
    - Mahalanobis distance between x and mean (origin) is $x^T C^{-1} x = x^T S^{-2} x$

Multivariate Gaussian

- Scaling and Rotating the coordinate frame
  - Let **Y := UX = USW**, where U is a rotation matrix that rotates the coordinate frame
    - Covariance matrix $C' = AA^T = (US)(US)^T = US^2U^T$
    - Mahalanobis distance, w.r.t. C', from **0** to $y:=Ux$ is $y^TC^{-1}y$ $= (Ux)^T (US^{-2}U^T) (Ux) = x^T S^{-2} x$
      = same as Mahalanobis distance, w.r.t. C, from **0** to x
    - Rotating data x simply rotates the iso-probability contours of P(X)

Multivariate Gaussian

- **Connections to PCA**
  - Let us apply **$A := USV^T$** to a **zero-mean isotropic Gaussian PDF**
  - (1) Rotation V^T doesn't change PDF
    - Covariance C = Identity
  - (2) Scaling S scales each dimension d by S_{dd} making the PDF anisotropic
    - Consider distinct $S_{11} > S_{22} > \ldots$
    - Covariance $C = S^2$
    - Variance is S_{dd}^2 along axis d (modes of variation = axes)
  - (3) Rotation U rotates the anisotropic PDF
    - Variance is S_{dd}^2 along U_d (modes of variation = U_d)
    - Covariance $C = US^2U^T$

Multivariate Gaussian

- Connections to PCA
  - Given: Data $\{x_i : i=1,\ldots,n\}$
  - Goal: Estimate modes of variation
  - Algorithm:
    1) Find maximum likelihood estimate (MLE) of covariance C
       - MLE for Gaussian mean is sample mean
       - MLE for Gaussian covariance is sample covariance
       - Consistent estimator
    2) Find eigen decomposition of C to give U and S:
       - Modes of variation U_i
       - Variance S_{ii}^2 along each mode of variation

Multivariate Gaussian

- **Directions of maximal variance**
  - Consider data $\{x_i : i=1,...n\}$ drawn from a Gaussian PDF with mean **$\mu = 0$ and <u>diagonal covariance</u> C**
  - For a Gaussian PDF, a diagonal covariance implies:
    - $X^d = (C_{dd})^{0.5} W^d$ where
      W^d is a standard Normal RV
  - Question:
    Find the direction / unit-vector v such that the data projected on the subspace denoted by vector v passing through the mean (origin) has maximal variance
  - Answer (derivation) follows

Multivariate Gaussian

- Directions of maximal variance
  - Projected data = $\langle x_i, v \rangle$ v
  - Mean of the projected data = $\Sigma_i \langle x_i, v \rangle$ v
    = $\langle \Sigma_i x_i, v \rangle$ v = $\langle 0, v \rangle$ v = 0
  - Projected data is 1D
  - Distance of projected data from the mean
    = $\|\langle x_i, v \rangle v\|_2 = |\langle x_i, v \rangle|$
  - Variance of projected data = $\Sigma_i \langle x_i, v \rangle^2$
  - Optimal direction $= \arg\max_{v:\|v\|_2=1} \sum_i \langle x_i, v \rangle^2$

Multivariate Gaussian

- Directions of maximal variance
  - Optimal direction

$$
\begin{aligned}
&= \arg\max_{v:\|v\|_2=1} \sum_i (x_i^T v)^2 \\
&= \arg\max_{v:\|v\|_2=1} \sum_i (x_i^T v)^T (x_i^T v) \\
&= \arg\max_{v:\|v\|_2=1} \sum_i v^T x_i x_i^T v \\
&= \arg\max_{v:\|v\|_2=1} v^T \left(\sum_i x_i x_i^T\right) v \\
&= \arg\max_{v:\|v\|_2=1} v^T C v
\end{aligned}
$$

    - where C = sample covariance
    - This is the connection between sample covariance C and direction v maximizing variance of projected data

Multivariate Gaussian

- Directions of maximal variance
  - Optimal direction

    $= \arg\max_{v:\|v\|_2=1} \sum_d C_{dd}(v^d)^2$

    - because C is diagonal
  - This is maximized when

    $v^d = 1$ for $d = \arg\max_e C_{ee}$ and $v^d = 0$ otherwise

    - Put all "weight" on that component of v that is associated with the maximum of diagonal elements in C
    - Constraint set = hypersphere.
      Contours of objective function are ellipsoids; minor axis = dimension corresponding to $\min_d (1/C_{dd})$ or $\max_d (C_{dd})$.
      Point, on hypersphere, maximizing objective function lies at intersection of minor axis with hypersphere

Multivariate Gaussian

- Directions of maximal variance
  - Question: Find 2nd direction u that is:
    - (i) orthogonal to v and
    - (ii) maximizes variance of data projected onto it
  - Optimal direction

$$= \arg\max_{u:\|u\|_2=1, u\perp v} \sum_i \langle x_i, u\rangle^2$$

$$= \arg\max_{u:\|u\|_2=1, u\perp v} \sum_d C_{dd}(u^d)^2, \text{ where we know } C_{dd} \geq 0$$

  - This is maximized when

$$u^c = 1 \text{ for } c = \arg\max_{d\neq e} C_{dd} \text{ and } u^c = 0 \text{ otherwise}$$

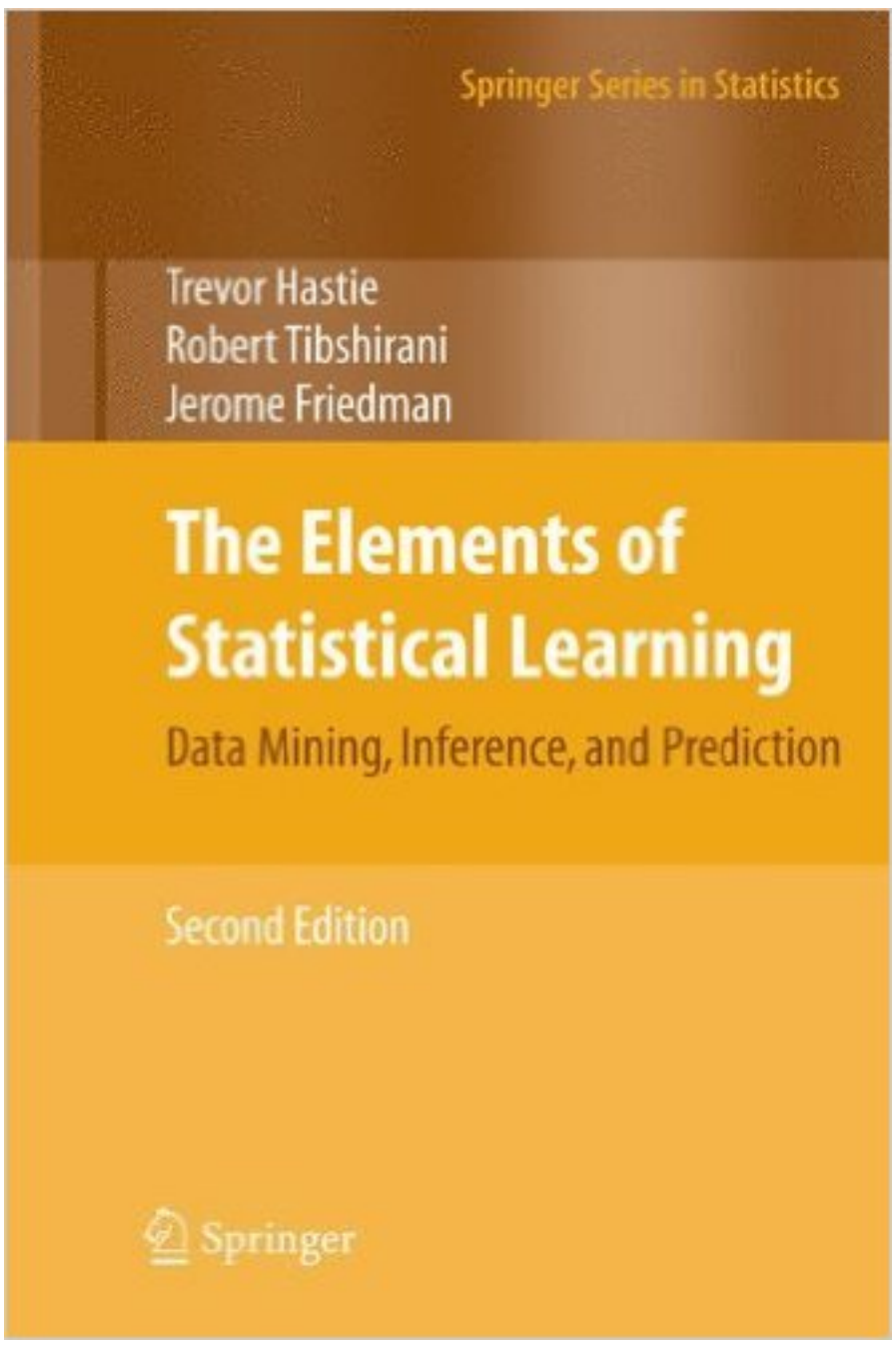
    - Put all "weight" on that component of u that is: (i) not the d chosen before and (ii) corresponds to the maximum of the remaining diagonal elements in C

Multivariate Gaussian

- Directions of maximal variance
  - Similar arguments hold for 3rd, 4th, … directions
  - Theorem:
    For data drawn from a Gaussian
    with mean 0 and a diagonal covariance matrix,
    the directions maximizing variance are
    the cardinal directions
  - These directions = **principal components of variation**
  - Rotating the coordinate frame by pre-multiplication with a orthogonal matrix U simply rotates the principal components

Multivariate Gaussian

- PCA and eigen decomposition
  - Theorem:
    The **principal directions** U for
    data that are observations of $X := AW + \mu$
    are the **eigenvectors** of the sample (empirical)
    covariance $C = AA^T$
  - **Variances** along principal directions are the **eigenvalues** of the sample (empirical) covariance matrix C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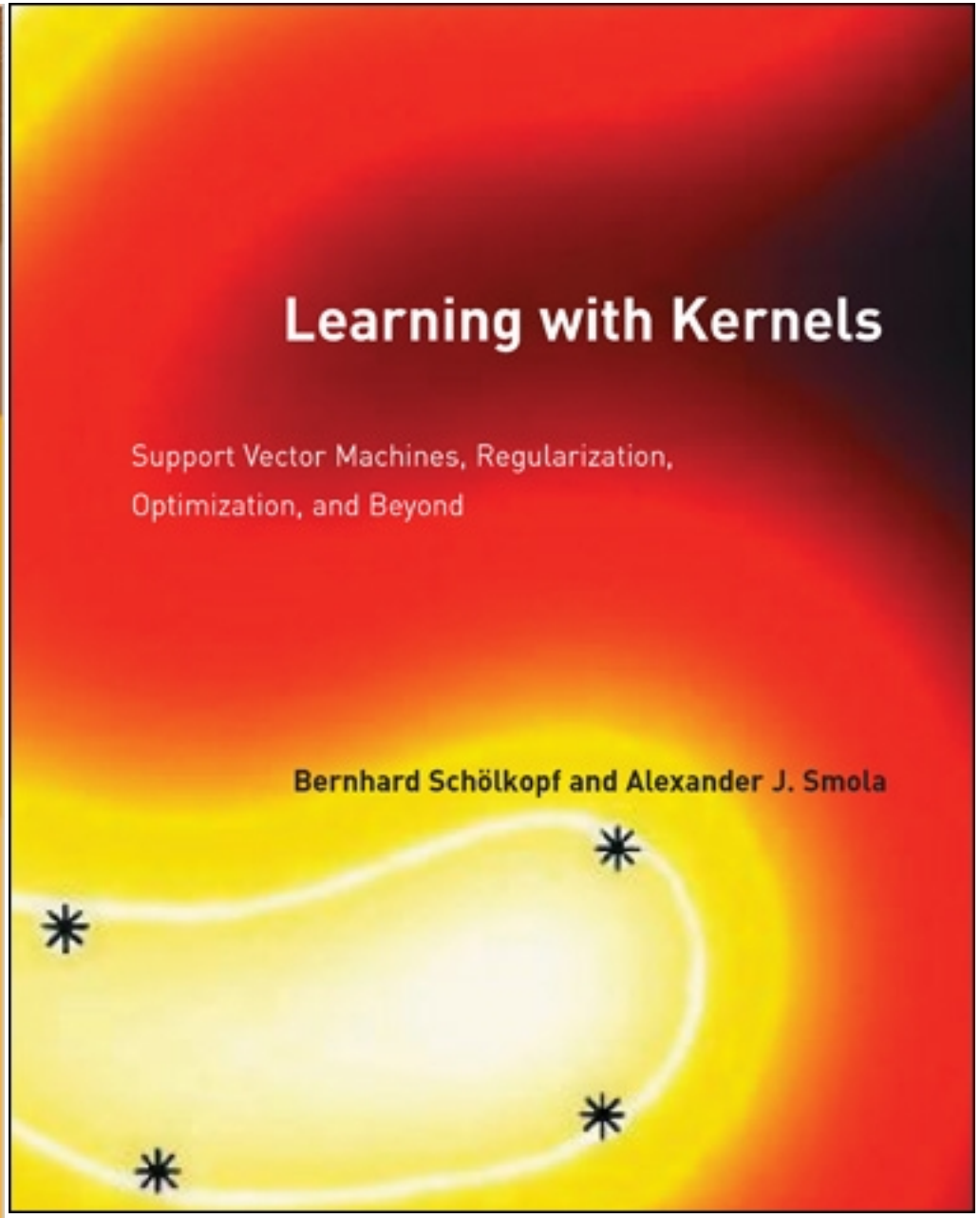
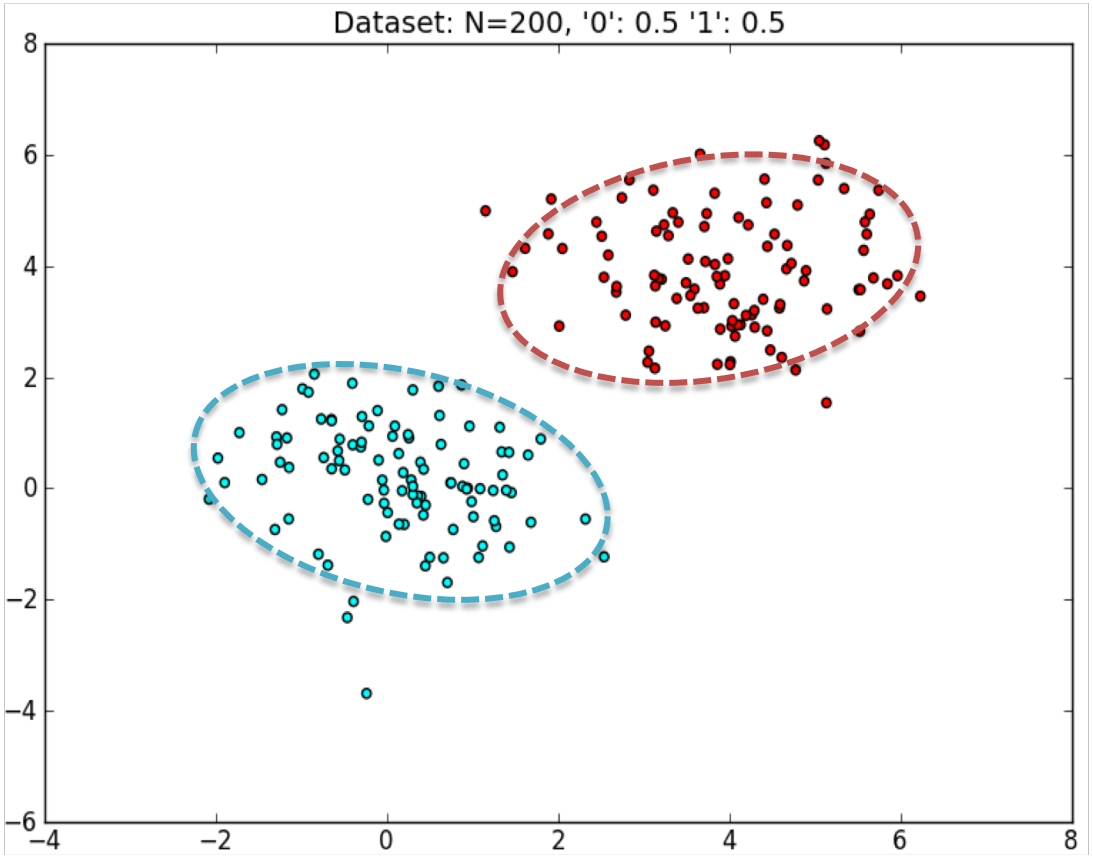

Learning with Kernels
Support Vector Machines, Regularization, Optimization, and Beyond
Bernhard Schölkopf and Alexander J. Smola

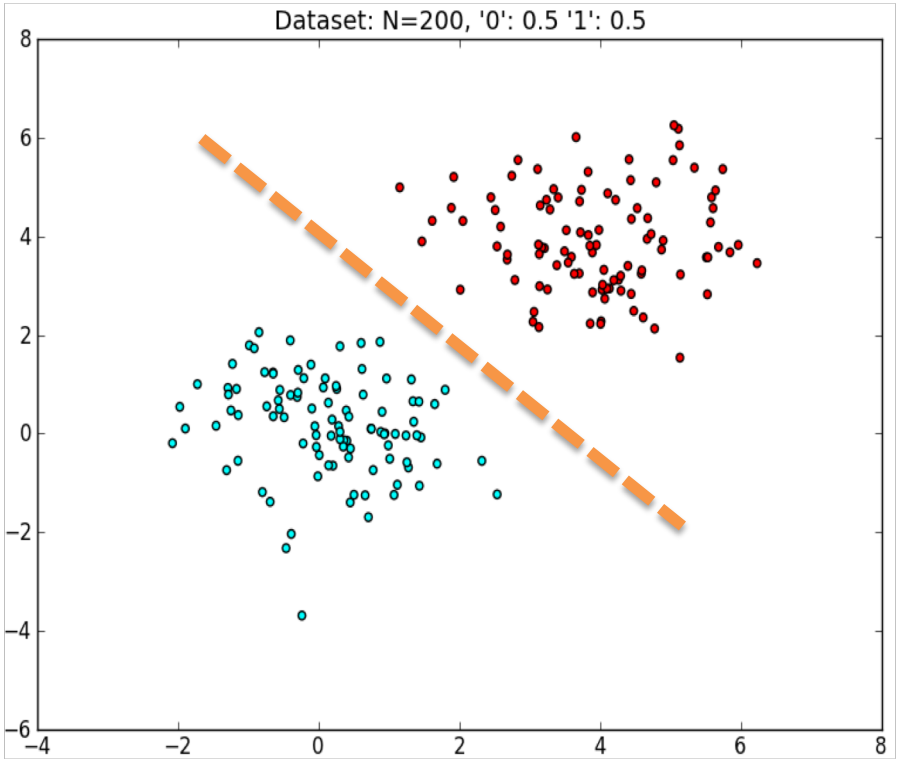
Modeling Data

- **Generative modeling**
  - Data in ellipsoidal clusters / classes
  - Use a Gaussian to model the data
  - How to classify ?
    - For a test point, assign point to cluster that gives larger probability



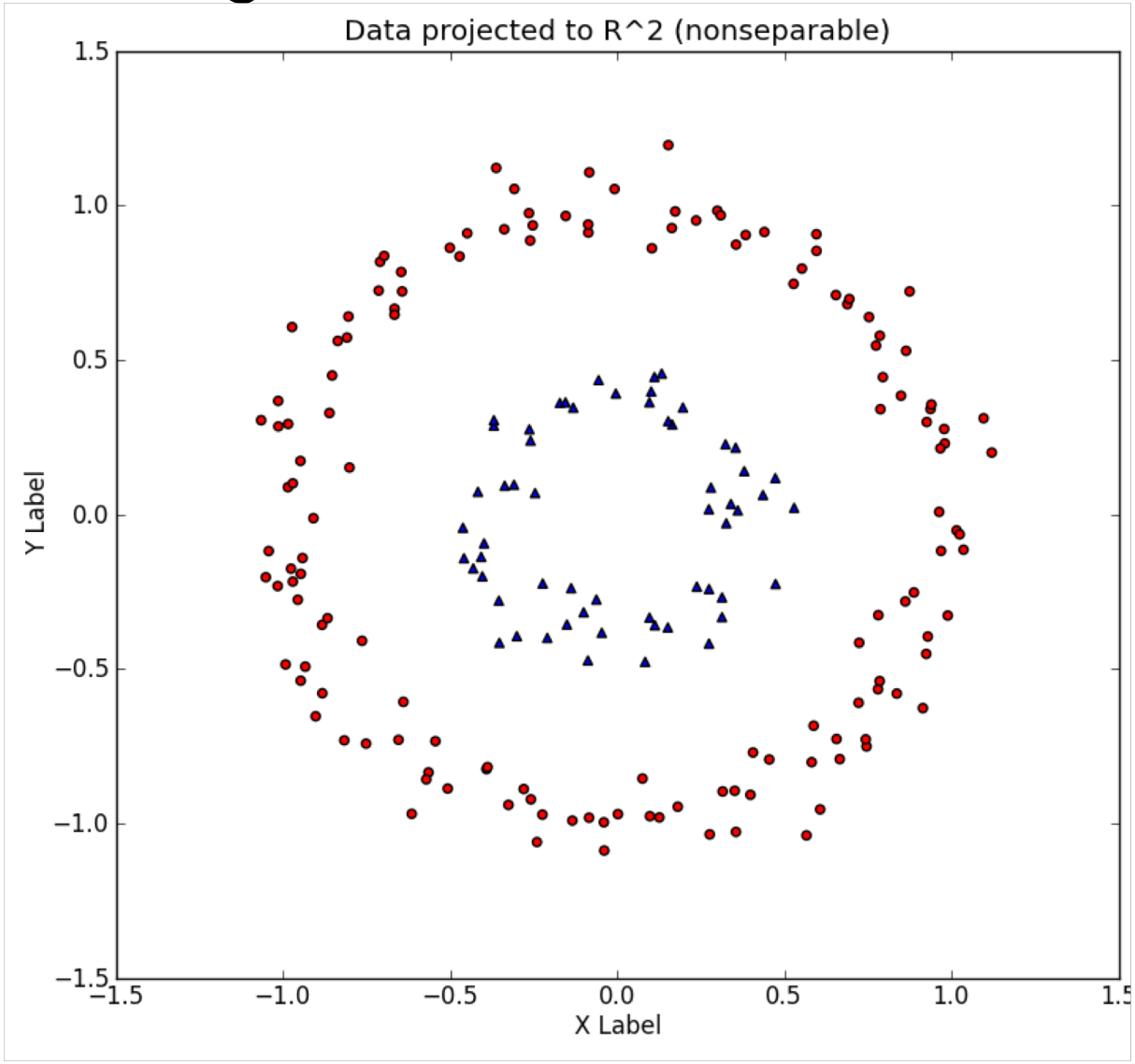
Modeling Data

- **Discriminative modeling** (for classification)
  - Data linearly separable
  - Use a line / plane to separate 2 classes
  - What if the data doesn't conform to this model ?



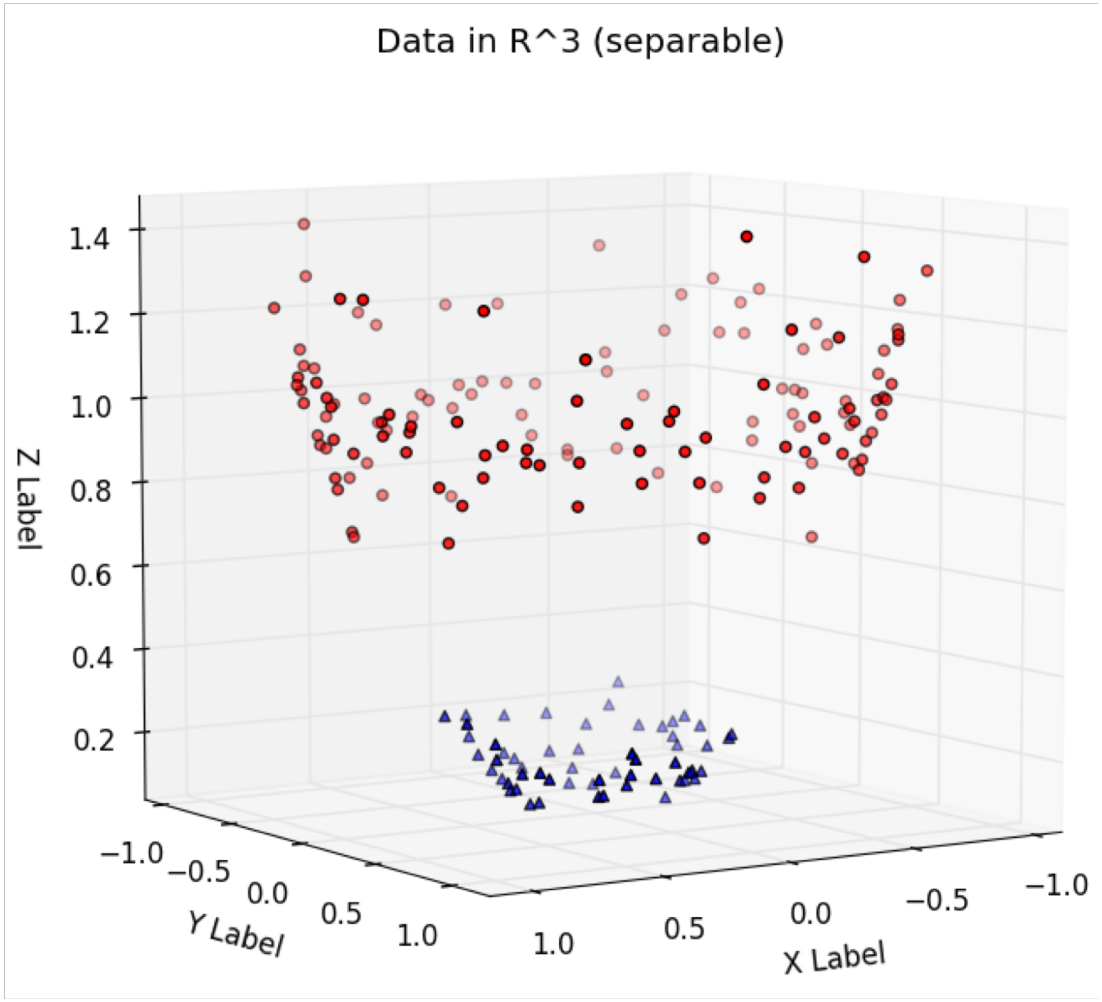
Modeling Complex Data

- Discriminative modeling (for classification)
- Example
  - Classes not linearly separable



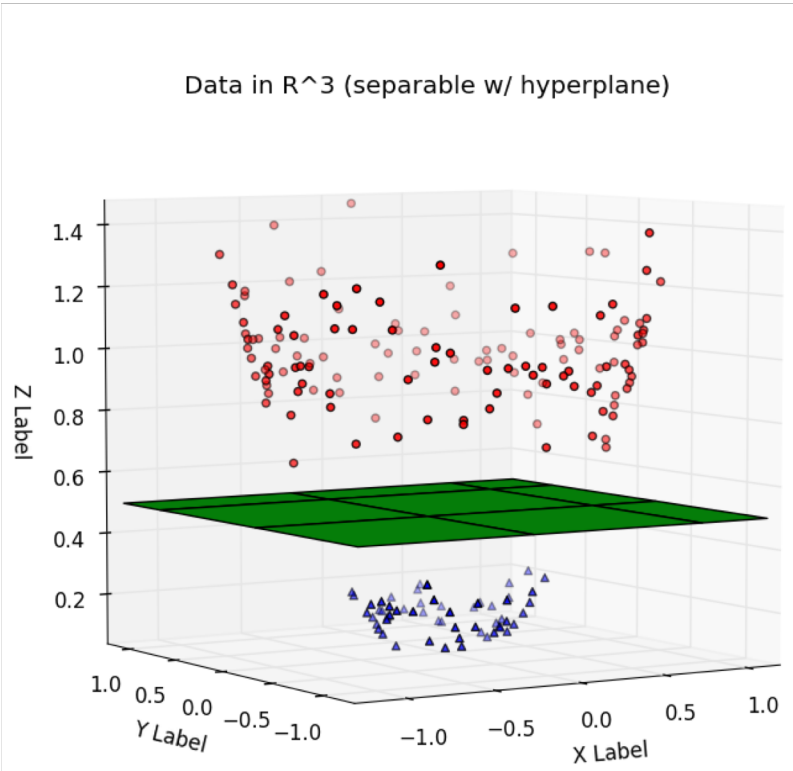
Modeling Complex Data

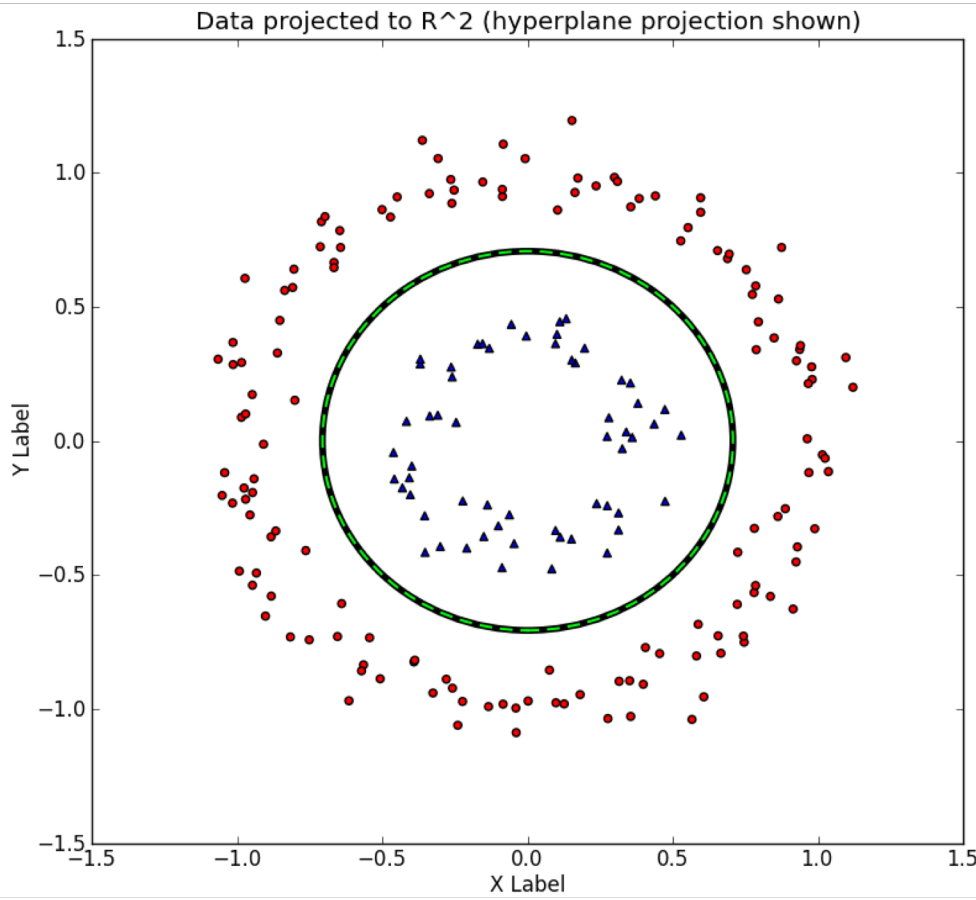
- Discriminative modeling (for classification)
  - Map [x, y] → [x, y, z := $x^2 + y^2$]



Modeling Complex Data

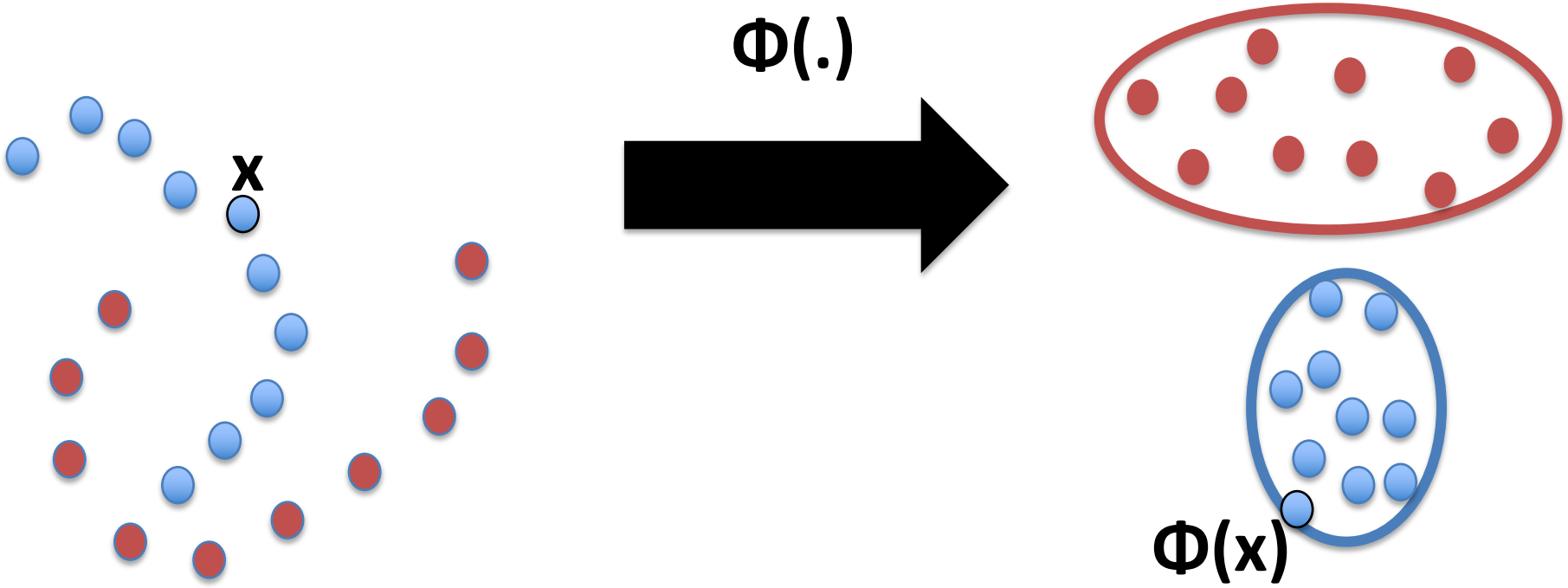
- Map [x, y] → [x, y, z := $x^2 + y^2$]
- In mapped space, data is linearly separable





Modeling Complex Data

- **Generative modeling**
  - Design a (nonlinear) mapping so that data becomes more Gaussian in the mapped space



Kernel Trick

- Mapped space can be very high dimensional
  - Datum = x, Mapped datum = $\Phi(x)$
- Mapping function $\Phi(.)$ can be very complex
- Don't work with mapped data explicitly
- Use a 'kernel' function
  - $k(x, y) = \langle \Phi(x), \Phi(y) \rangle$
  - Kernel gives the inner product in mapped space
  - Don't store $\Phi(x)$ at all
  - Use k(x,y) for all computations
- Identity map $\Phi(.)$ => $k(x,y) = \langle x,y \rangle$

Kernel Trick

- Each mapping function equivalent to a kernel
- In practice, we choose a kernel first !
- Some theorems describe conditions on the kernel for the existence of an equivalent map
  - e.g., k(x,y) = exp (a $||x-y||^2$); a = free parameter
    - Gaussian / Radial basis function (RBF) kernel
  - Mapped space has infinite dimension

$$\exp\left(-\frac{1}{2}||\mathbf{x}-\mathbf{x}'||^2\right) = \sum_{j=0}^{\infty} \frac{(\mathbf{x}^\top \mathbf{x}')^j}{j!} \exp\left(-\frac{1}{2}||\mathbf{x}||^2\right) \exp\left(-\frac{1}{2}||\mathbf{x}'||^2\right)$$

    - e.g., for degree j = 2, points x=[x1,x2], y=[y1,y2] in 2D:

$$(\mathbf{x}\cdot\mathbf{y})^2 = (x_1^2, x_1x_2, x_2x_1, x_2^2)(y_1^2, y_1y_2, y_2y_1, y_2^2)^\top$$

Kernel Trick

- Hilbert space
  - Vector space having the structure of an inner product
  - Inner product allows us to measure:
    - Distances / lengths, via the induced norm
    - Angle between two vectors
  - Inner-product function satisfies properties of:
    - Symmetry
    - Linearity in first argument
    - Positive definiteness

Kernel Trick

- **Reproducing kernel**

Definition 2 (Reproducing Kernel). *Let $\mathcal{H}$ be a Hilbert space of functions $f : \mathcal{X} \longrightarrow \mathbb{R}$ defined on a non-empty set $\mathcal{X}$. A function $k : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$ is called a reproducing kernel of $\mathcal{H}$ if it satisfies*

(1) $\forall x \in \mathcal{X}, k_x = k(x, \cdot) \in \mathcal{H}$,

(2) $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f, k_x \rangle_{\mathcal{H}} = f(x)$ *(the reproducing property).*

In particular, for any $x, y \in \mathcal{X}$, $k(x, y) = \langle k_x, k_y \rangle_{\mathcal{H}} = \langle k_y, k_x \rangle_{\mathcal{H}} = k(y, x)$.

  - Kernel is *representor of evaluation* (or, *evaluation functional*)

- **Reproducing kernel Hilbert space**

Theorem 3. *A Hilbert space $\mathcal{H}$ is a reproducing kernel Hilbert space if and only if it has a reproducing kernel.*

Theorem 4. *If it exists, reproducing kernel is unique. Equivalently, a reproducing kernel Hilbert space uniquely determines its reproducing kernel.*

  - Evaluation functionals are bounded, continuous

Kernel Trick

- **Kernel**

Definition 3 (Kernel). *A function* $k : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$ *is called a kernel on* $\mathcal{X}$ *is there exists a Hilbert space (not necessarily a reproducing kernel Hilbert space)* $\mathcal{F}$ *and a map* $\mathbf{\Phi} : \mathcal{X} \longrightarrow \mathcal{F}$ *such that* $k(x, y) = \langle \mathbf{\Phi}(x), \mathbf{\Phi}(y) \rangle_{\mathcal{F}}$.

- Corollary:
  Every reproducing kernel is a kernel

Kernel Trick

- **Positive definite function**

Definition 4. *A symmetric function* $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *is positive definite if* $\forall n \in \mathbb{N}$, $\forall (a_1, \ldots, a_n) \in \mathbb{R}^n$ *and* $\forall (x_1, \ldots, x_n) \in \mathcal{X}^n$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j k(x_i, x_j) \geq 0.$$

The function $k(\cdot, \cdot)$ *is strictly positive definite if for mutually distinct* x_i*, the equality holds only when all the* a_i *are zero.*

- Corollary:
  Every kernel is a positive definite function

Kernel Trick

- **Moore-Aronszajn Theorem**

Theorem 5 (Moore-Aronszajn). *Let $k : \mathcal{X} \times \mathcal{X} \longrightarrow \mathbb{R}$ be positive definite. Then there is a unique reproducing kernel Hilbert space with reproducing kernel k. In particular, the span of the reproducing kernel k is dense in the resulting reproducing kernel Hilbert space.*

  - Key construction: H is completion of H_0, where

Let the space $\mathcal{H}_0 = \text{span}\{k(x, \cdot) : x \in \mathcal{X}\}$ be endowed with the inner product

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j k(x_i, y_j),$$

where $f = \sum_{i=1}^{n} \alpha_i k(x_i, \cdot)$ and $g = \sum_{j=1}^{m} \beta_j k(y_j, \cdot)$

  - Inner product is:
    - Linear: <u+v,w>=<u,w>+<v,w> & <au,v>=a<u,v>, by construction
    - Symmetric: <u,v>=<v,u>, **because k(.,.) is symmetric**
    - Non-degenerate: **because k(.,.) is positive definite;** <u,u> >=0 and <u,u> =0 iff u=0

Kernel Trick, Density Estimation

- Consider mean of mapped data

$$\mathbf{\Phi}_0 = 1/n \sum_{i=1}^{n} \mathbf{\Phi}(\mathbf{x}_i)$$

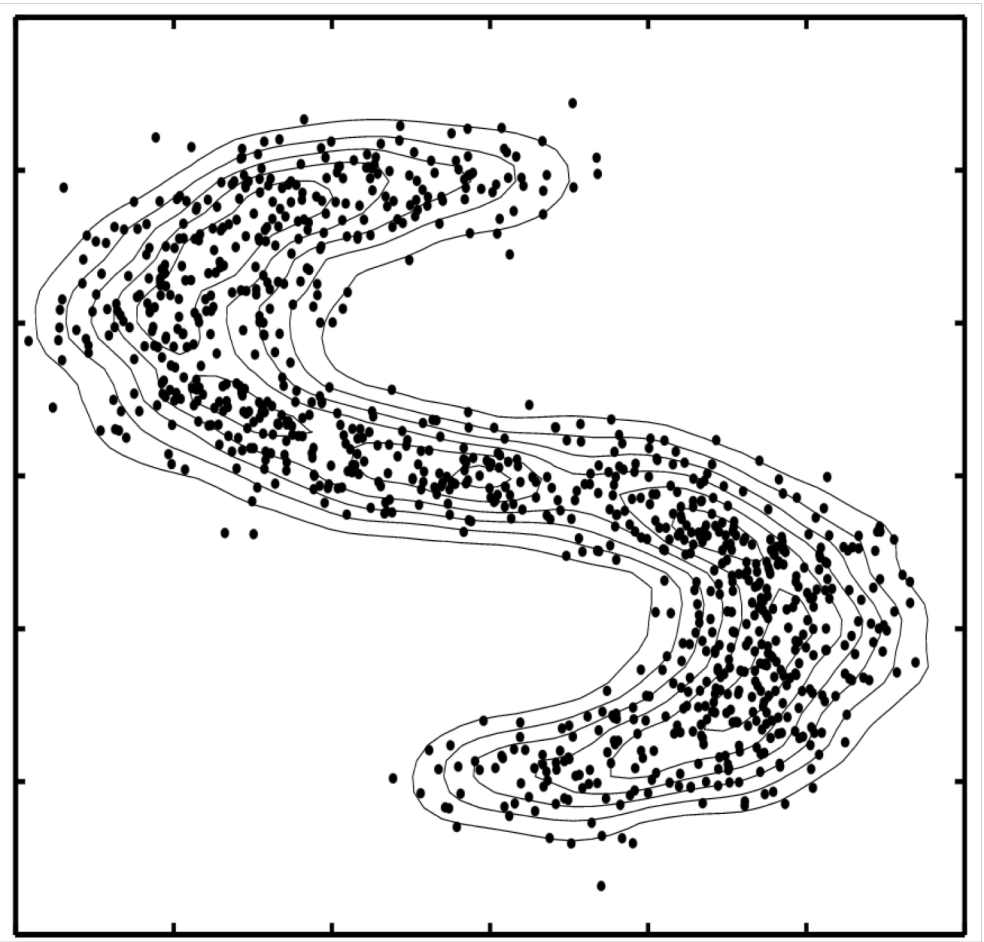
- Distance between mapped datum and mean

$$\|\mathbf{\Phi}(\mathbf{z}) - \mathbf{\Phi}_0\|^2 = k(\mathbf{z}, \mathbf{z}) - \frac{2}{n} \sum_{i=1}^{n} k(\mathbf{z}, \mathbf{x}_i) + \frac{1}{n^2} \sum_{i,j=1}^{n} k(\mathbf{x}_i, \mathbf{x}_j)$$

  - 3rd term = constant ⟶ ignore
  - 1st term = constant for RBF kernel ⟶ ignore
  - 2nd term equivalent to using density estimation using RBF (Gaussian) mixture model
    - Larger probability ⟶ closer to mean

Kernel Trick, Density Estimation

$$\sum_{i=1}^{n} k(\mathbf{z}, \mathbf{x}_i)$$



- How do its contours look like ?
  - Contours adapt to the nonlinear distribution of the data
  - Without kernels (with 1 isotropic Gaussian), contours will be circular, not adapted to data

Principal Component Analysis

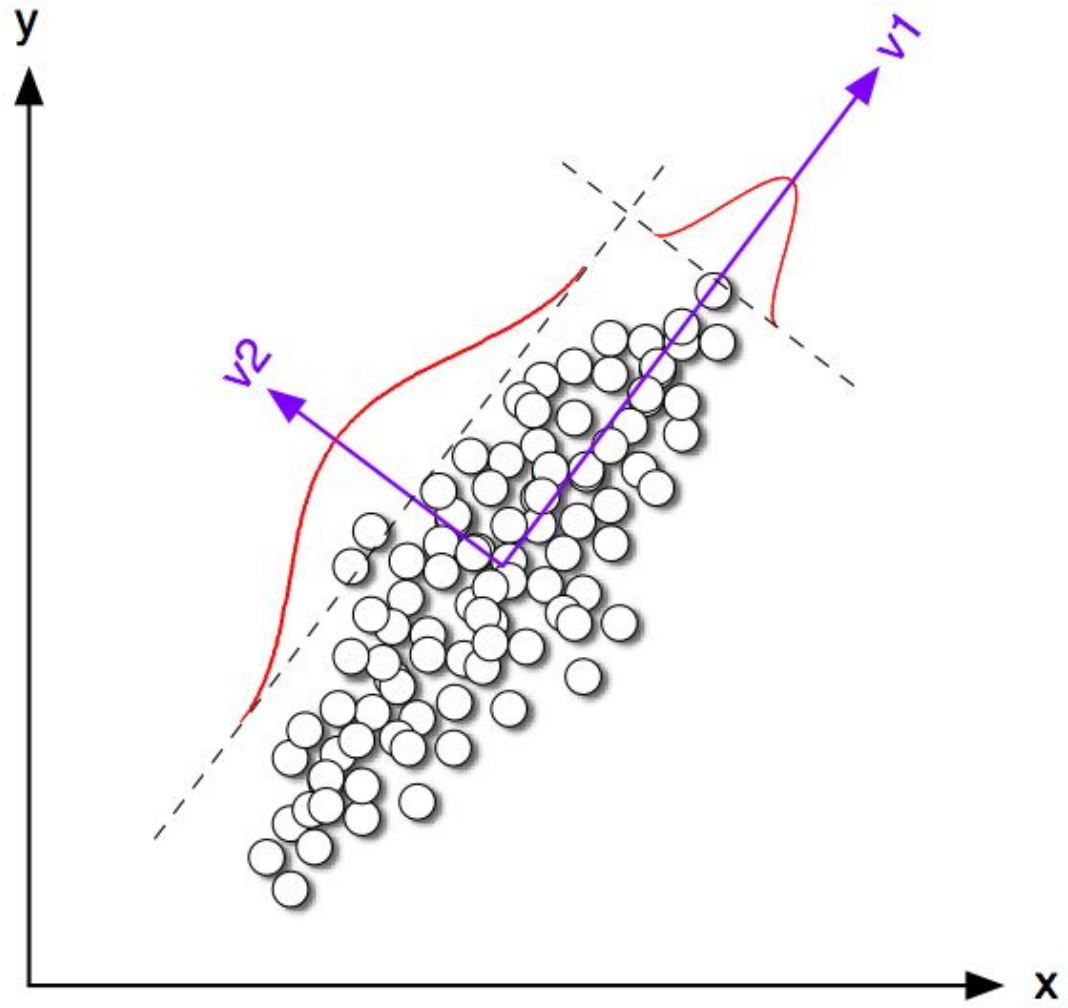
- Data sample = $\{x_j\}$
- Mean estimate = sample mean
- Now, considered centered data
  - Shift in coordinate frame
- Covariance estimate = sample covariance
  - Covariance matrix $C = \frac{1}{M}\sum_{j=1}^{M} \mathbf{x}_j \mathbf{x}_j^\top$
- Eigenvectors of C → directions of variation

$\lambda \mathbf{v} = C\mathbf{v}$ = $\frac{1}{M}\sum_{j=1}^{M}(\mathbf{x}_j \cdot \mathbf{v})\mathbf{x}_j$

  - All eigenvectors must lie in the span of data

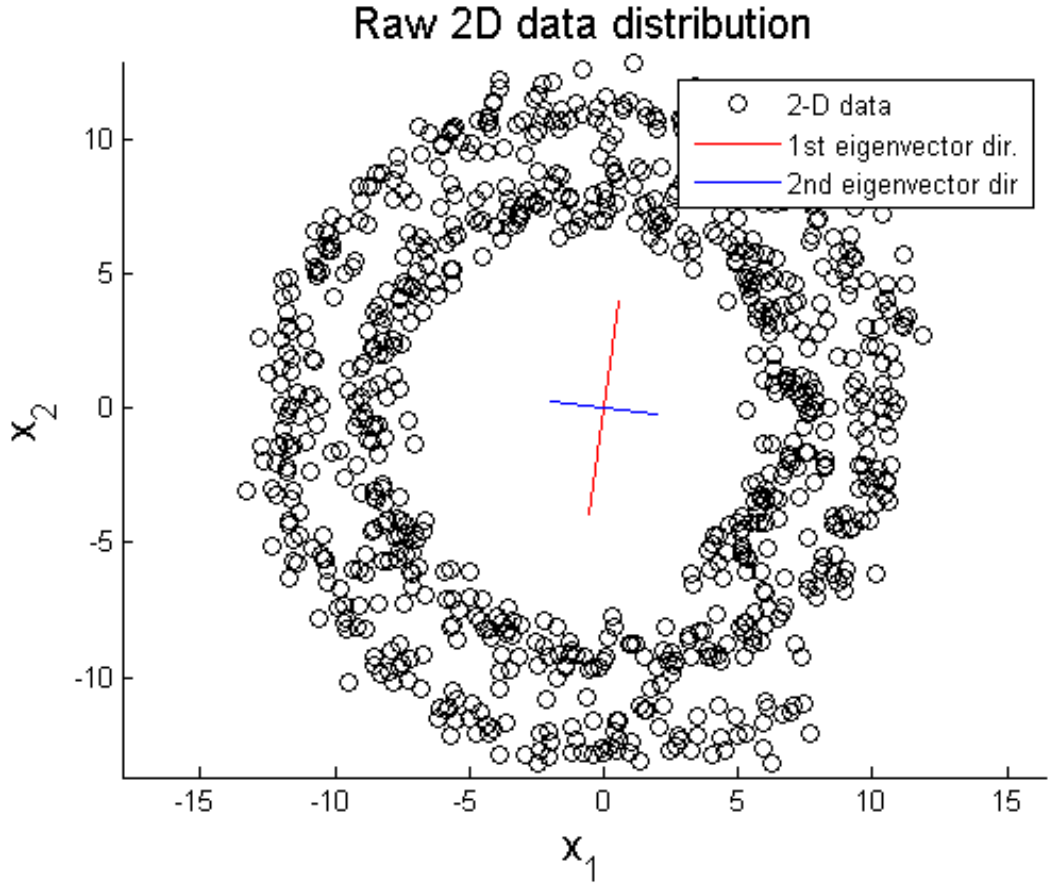
PCA

- PCA for Gaussian distributed data



PCA

- But PCA doesn't work well for a data cluster that isn't ellipsoidal
  - e.g., what if data has the following distribution ?



Kernel PCA

- For centered data, covariance matrix is:

$$\bar{C} = \frac{1}{M} \sum_{j=1}^{M} \Phi(\mathbf{x}_j) \Phi(\mathbf{x}_j)^\top$$

- We can model eigenvector V as $\mathbf{V} = \sum_{i=1}^{M} \alpha_i \Phi(\mathbf{x}_i)$

- For eigenvector V: $\lambda \mathbf{V} = \bar{C} \mathbf{V}$
  - Take inner product with one of the $\Phi(x_k)$

$$\lambda(\Phi(\mathbf{x}_k) \cdot \mathbf{V}) = (\Phi(\mathbf{x}_k) \cdot \bar{C}\mathbf{V})$$

- Substituting forms of V and C in this equation, we get, for each k, …

Kernel PCA

- This can be simplified to $M\lambda K\boldsymbol{\alpha} = K^2\boldsymbol{\alpha}$ where K = Gram matrix for centered data s.t. $K_{ij} := (\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)),$
- Solve: $M\lambda\boldsymbol{\alpha} = K\boldsymbol{\alpha}$
  - All solutions α satisfy previous equation
  - Additional solutions α won't lead to difference in 'v'
- Eigenvectors of K give vectors α that in turn represent V (need to normalize to unit norm)
- λ = eigenvalues of covariance matrix
  = (1/M) eigenvalues of K

Kernel PCA

- Linear modes in mapped space -> nonlinear modes of variation in input space
  - Call 'feature' = < Φ(x), v >
  - Visualize contours of feature values over domain

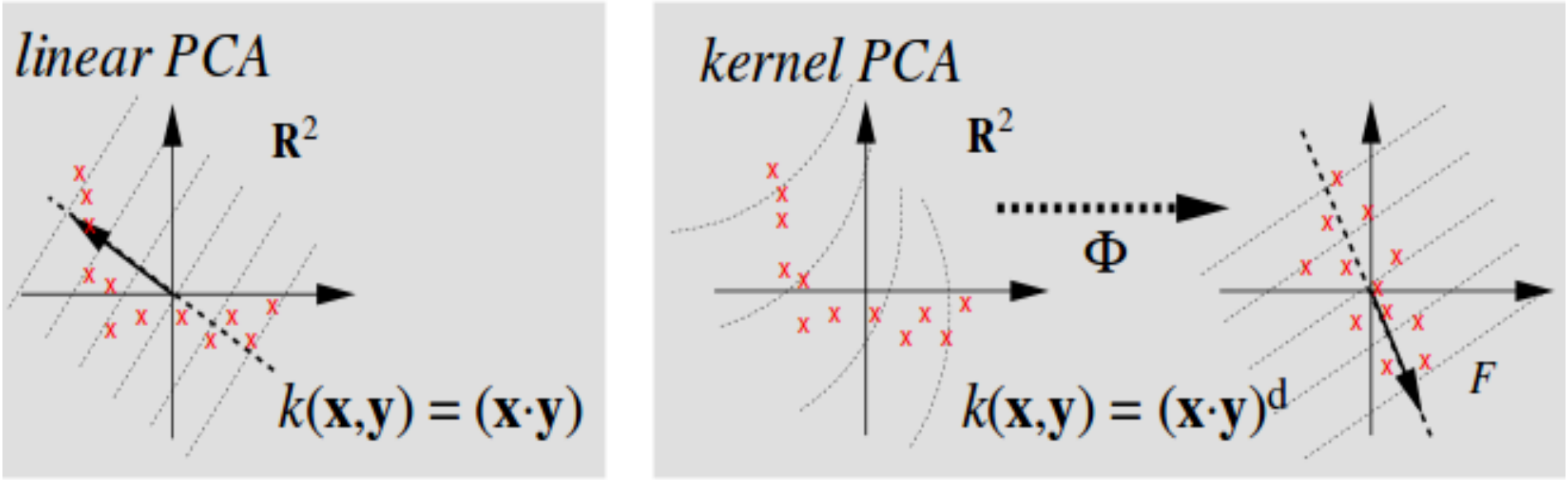


Fig. 1. Basic idea of kernel PCA: by using a nonlinear kernel function k instead of the standard dot product, we implicitly perform PCA in a possibly high–dimensional space F which is nonlinearly related to input space. The dotted lines are contour lines of constant feature value.

KPCA

- Plot contour for constant distance from subspace selected by few principal eigenvectors
  - Can be better than GMM
  - Kernel choice matters

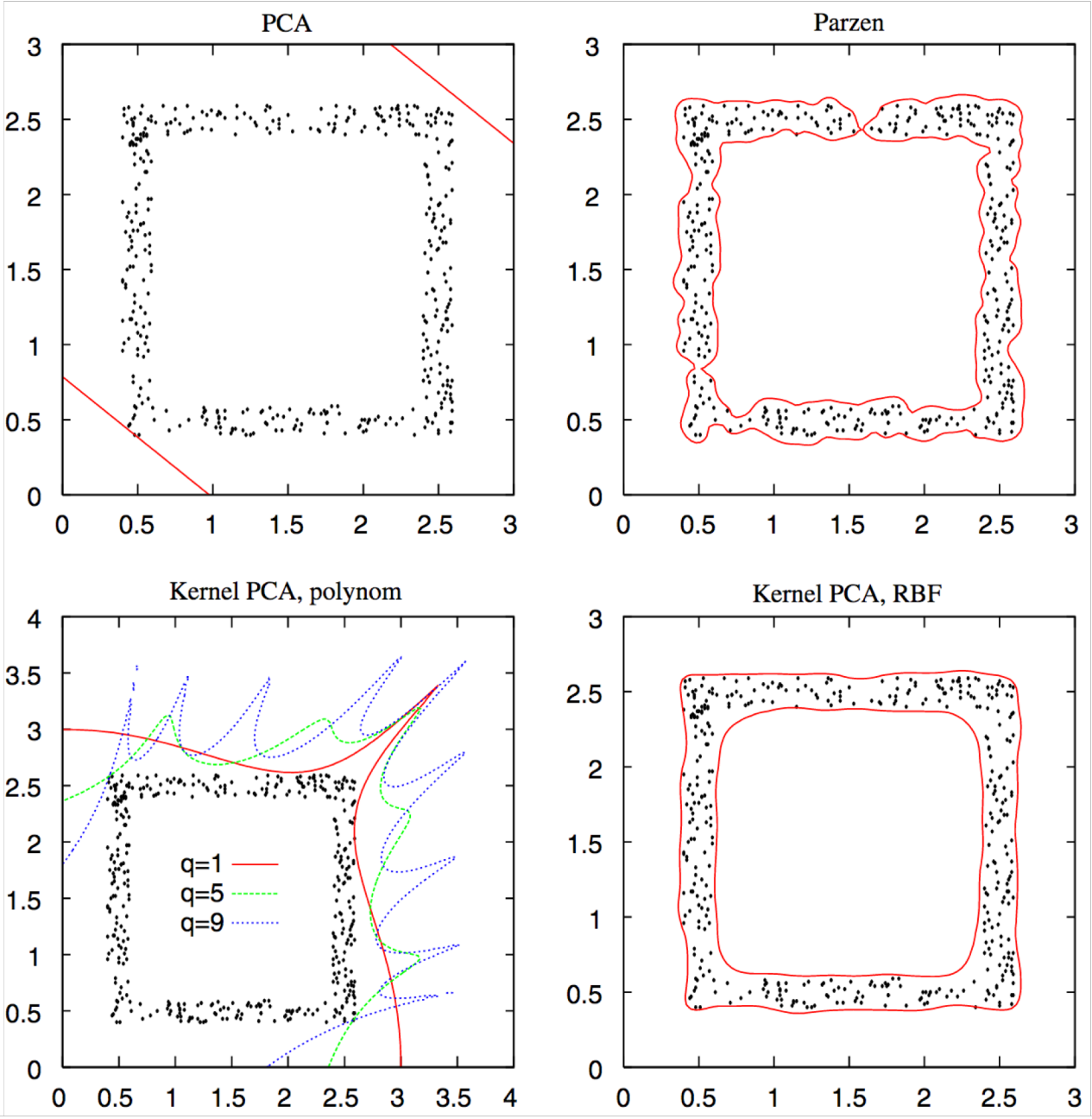
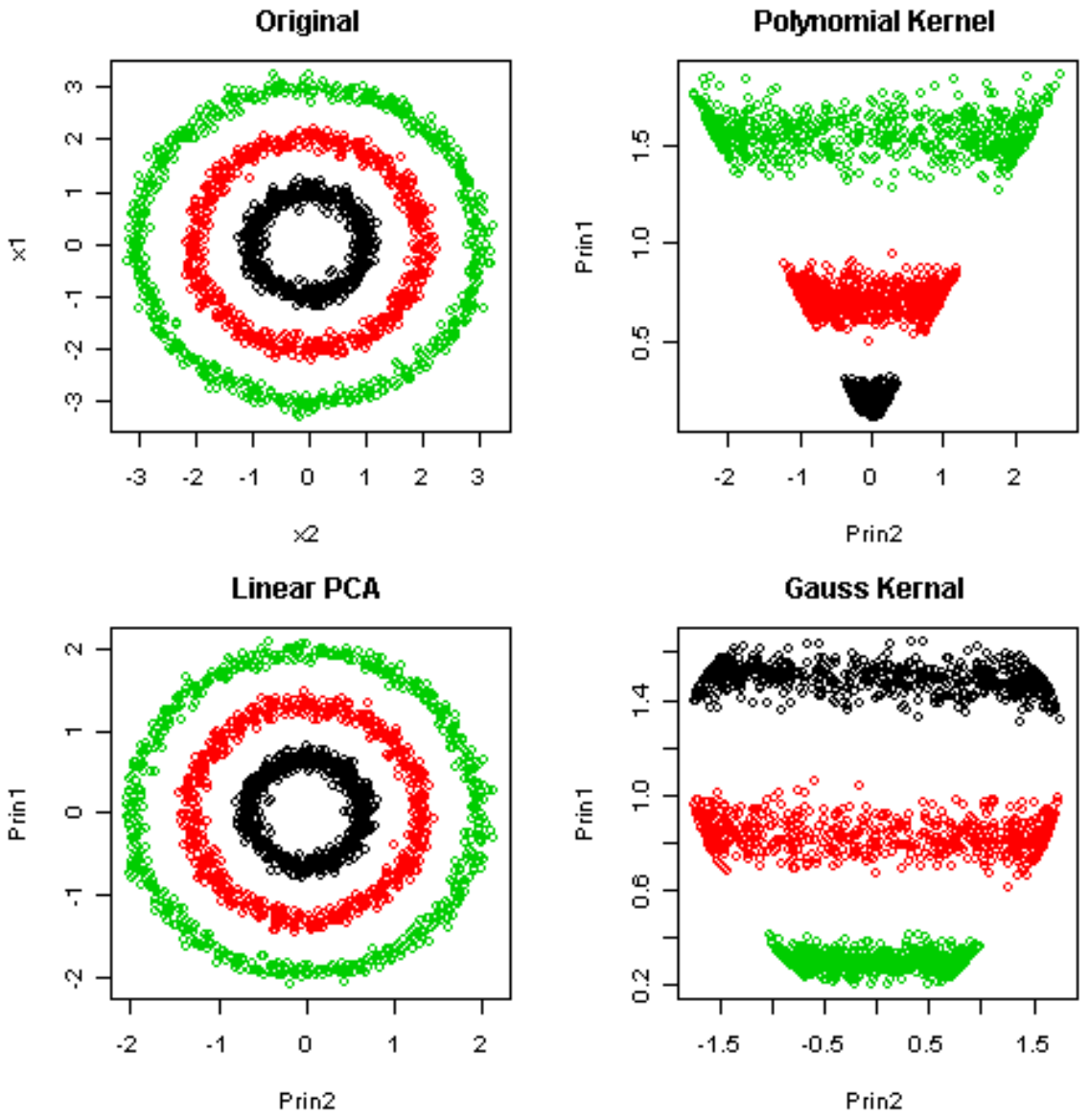


Fig. 2. Decision boundaries for various methods: (top left) PCA reconstruction error with $q = 1$ eigenvector, (top right) Parzen window density estimator with $\sigma = 0.05$, (bottom left) reconstruction error in $\mathcal{F}$ with polynomial kernel $k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i \cdot \mathbf{x}_j)^{10}$ and various q values, (bottom right) reconstruction error in $\mathcal{F}$ with Gaussian kernel using $\sigma = 0.4$ and $q = 40$.

Kernel PCA

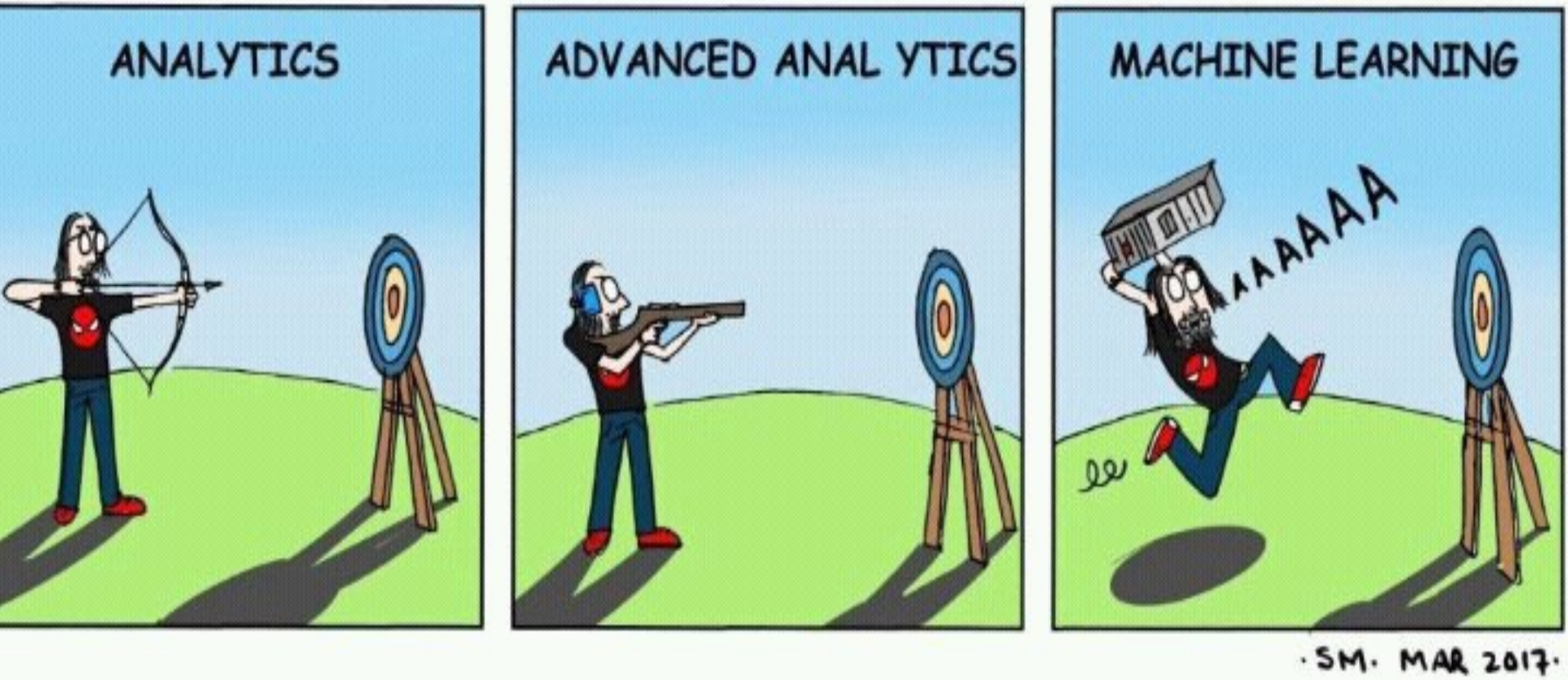
- More examples



- Preferred parameter-tuning method:
  "Grad student descent" =
  Grad student fiddles with parameters until it works
  [Ryan Adams, Harvard]

Data scientist = "Person who is better at statistics than any software engineer and better at software engineering than any statistician." [Josh Wills, Cloudera]

Data scientist = "Person who is worse at statistics than any statistician and worse at software engineering than any software engineer." [Will Cukierski, Kaggle]



"You've been traded for some big data,
two spreadsheets, and an algorithm."