DIMENSIONALITY REDUCTION AND VISUALIZATION

Loose ends from HW2

- Hyperparameters, bin size = 5, 10, 40, 100… ?
  - Tune on test set error rate
- Variance of a recognizer
  - Accuracy 100%? 98? 90? 80?
  - What's the mean and variance of the accuracy?
- A majority class baseline
  - Powerful if one class dominates
  - Recognizer becomes biased towards the majority class (the prior term)
  - Often happens in real life
  - How to deal with this?

Loose ends from HW2

- What happens to P(x | leave), if there’s no leave in the bin?
  - MLE estimates says P(a < x < b | leave) = 0
  - 0 probability for the entire term
  - Is this due to a bad sampling of the training set?
  - Can solve with MAP

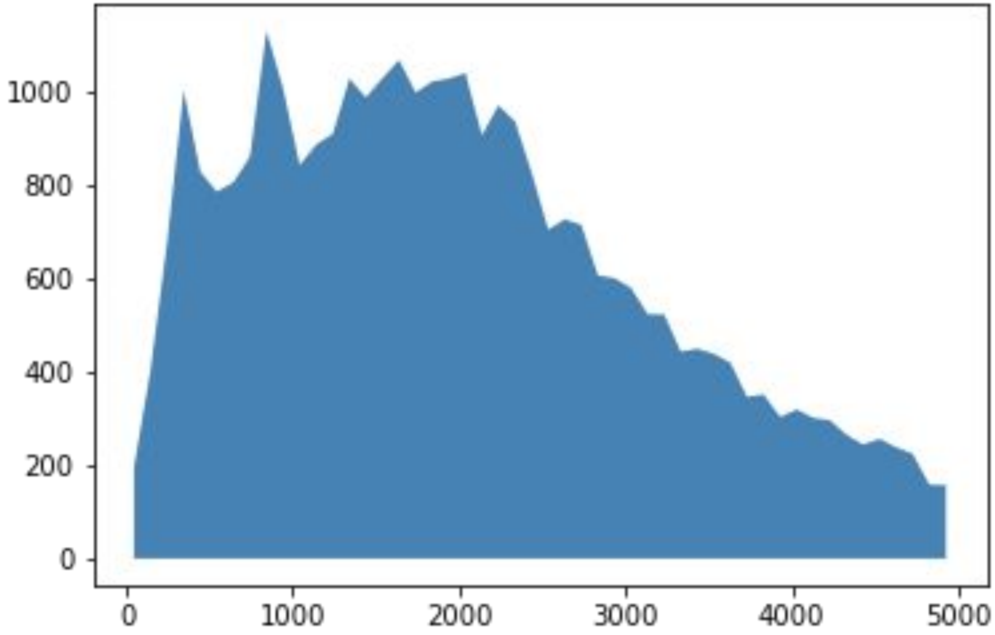
Map of a coin toss
β, α are prior
hyperparameters

$$\theta = \frac{k + \alpha - 1}{n + \alpha + \beta - 2}$$

  - Use unsupervised data for the priors?

Loose ends from HW2

- Another method to combat zero counts is to use Gaussian mixture models
  - How to select the number of mixtures?
    - Maybe all these can be a course project



ML Methodology

- Re-train using the full set for deployment (using the hyperparameters tuned on test)

- But you should have a real test set to evaluate this
  - Kaggle submission
  - Held out data

Train set: learn parameters
Validation/dev set: learn hyper parameters
Test set: evaluate

Evaluating a detection problem

- 4 possible scenarios

		Detector	
		Yes	No
Actual	Yes	True positive	False negative (Type II error)
	No	False Alarm (Type I error)	True negative

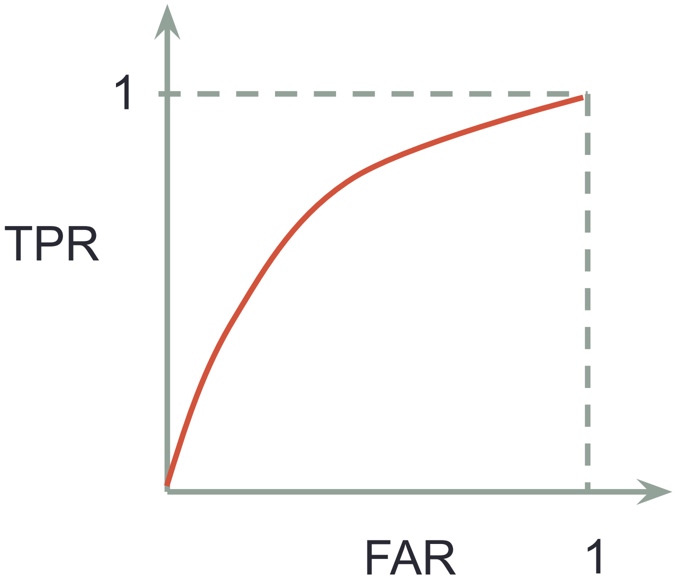
True positive + False negative = # of actual yes

False alarm + True negative = # of actual no

- False alarm and True positive carries all the information of the performance.

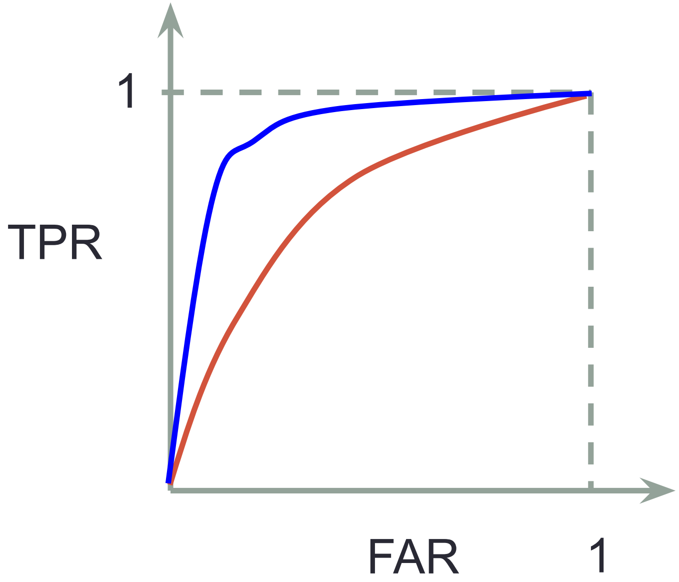
Receiver operating Characteristic (RoC) curve

- What if we change the threshold
- FA TP is a tradeoff
- Plot FA rate and TP rate as threshold changes



Comparing detectors

- Which is better?



Comparing detectors

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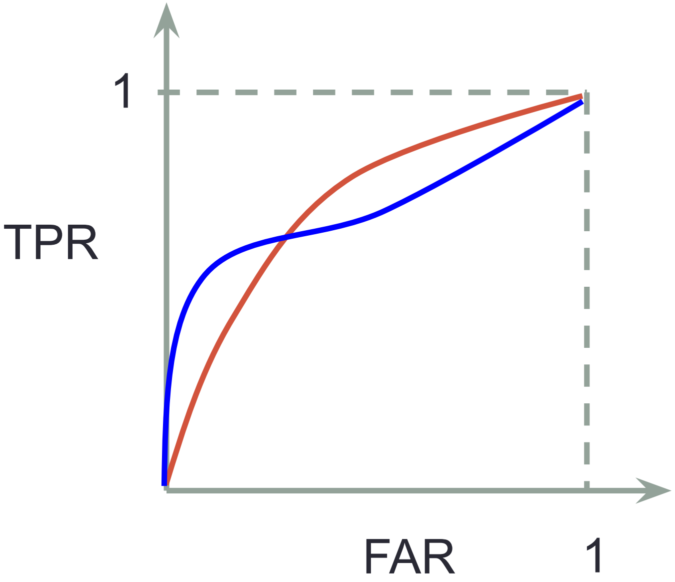
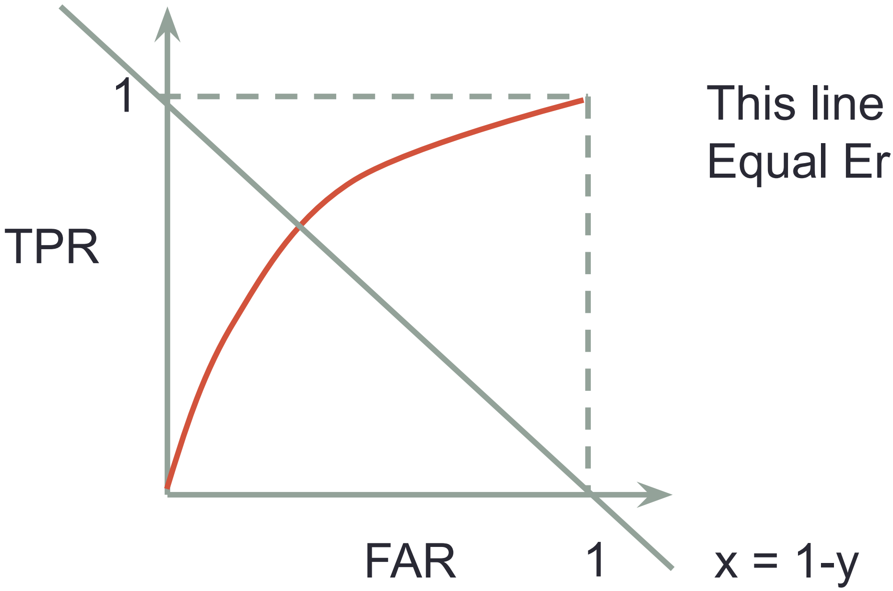


Selecting the threshold

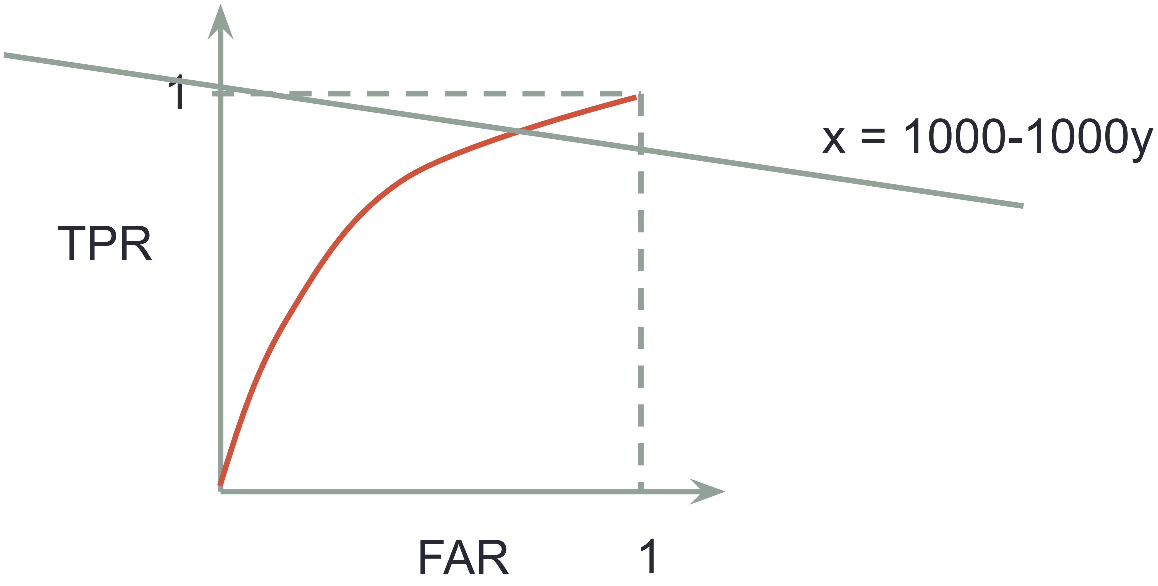
- Select based on the application
- Trade off between TP and FA. Know your application, know your users.
  - A miss is as bad as a false alarm   FAR = 1-TPR => x = 1-y



This line has a special name
Equal Error Rate (EER)

Selecting the threshold

- Select based on the application
- Trade off between TP and FA. Know your application, know your users. Is the application about safety?
  - A miss is 1000 times more costly than false alarm.
    - FAR = 1000(1-TPR) => x = 1000-1000y



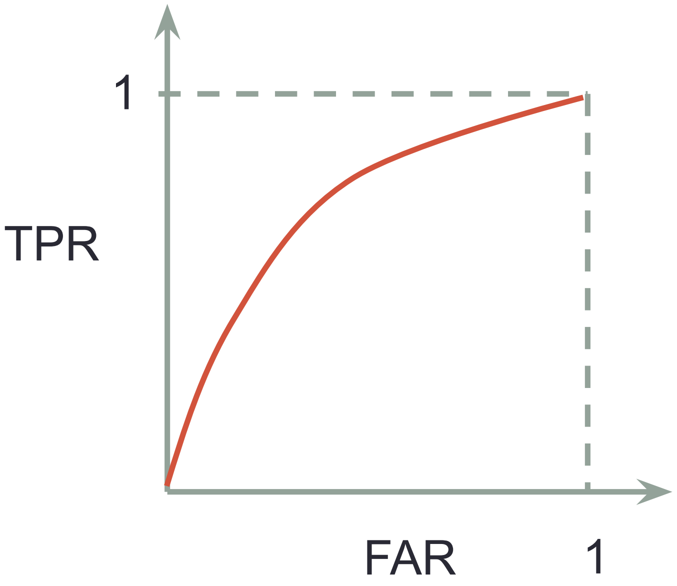
Churn prediction

Predict whether a customer will stop subscription, so we can send a promotional ad

Subscription fee 50

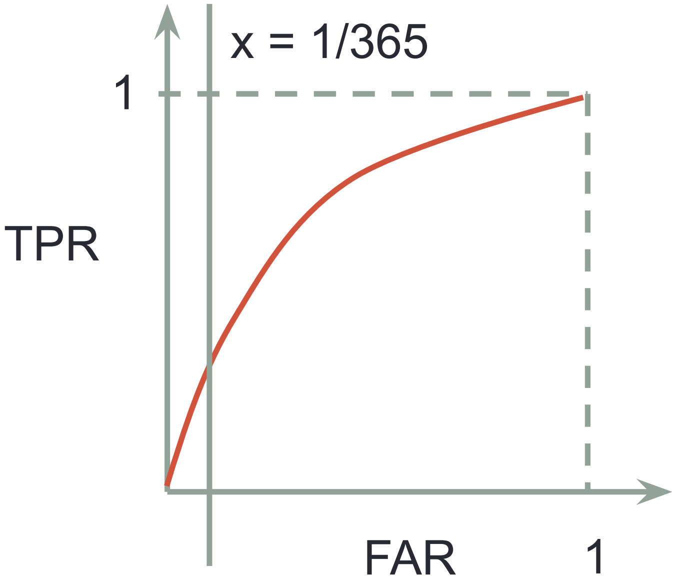
Promotional subscription fee 25

Where should I pick the threshold?

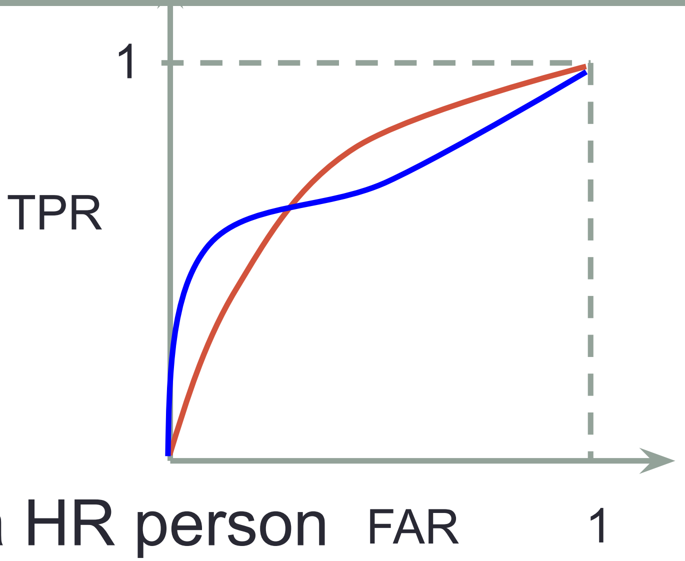


Selecting the threshold

- Select based on the application
- Trade off between TP and FA.
  - Regulation or hard threshold
  - Cannot exceed 1 False alarm per year
    - If 1 decision is made everyday, FAR = 1/365



Comparing detectors



- Which is better?

- You want to give your findings to a HR person so that he will conduct an interview with the person which detector to pick?

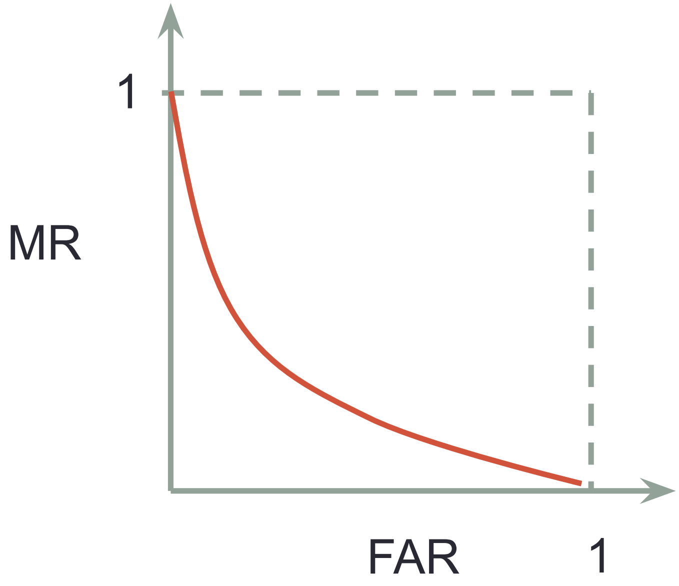
Interpretability

HR asks what can they do better.

What should you tell them based on your model?

Notes about RoC

- Ways to compress RoC to just a number for easier comparison -- use with care!!
  - EER
  - Area under the curve
  - F score
- Other similar curve - Detection Error Tradeoff (DET) curve
  - Plot False alarm vs Miss rate
- Can plot on log scale for clarity



DIMENSIONALITY REDUCTION AND VISUALIZATION

Mixture models

$$p(x) = \sum_k p(k)p_k(x)$$

- A mixture of models from the same distributions (but with different parameters)
- Different mixtures can come from different sub-class
  - Cat class
    - Siamese cats
    - Persian cats
- p(k) is usually categorical (discrete classes)
- Usually the exact class for a sample point is unknown.
  - Latent variable

EM on GMM

- E-step
  - Set soft labels: $w_{n,j}$ = probability that nth sample comes from jth mixture p
  - Using Bayes rule
    - p(k|x ; μ, σ, ϕ) = p(x|k ; μ, σ, ϕ) p(k; μ, σ, ϕ) / p(x; μ, σ, ϕ)
    - p(k|x ; μ, σ, ϕ) α p(x|k ; μ, σ, ϕ) p(k; ϕ)

$$p(k_n = j | x_n; \phi, \mu, \Sigma) = \frac{p(x_n; \mu_j, \sigma_j) p(k_n = j; \phi)}{\Sigma_l p(x_n; \mu_l, \sigma_l) p(k_n = l; \phi)}$$

EM on GMM

- M-step (soft labels)

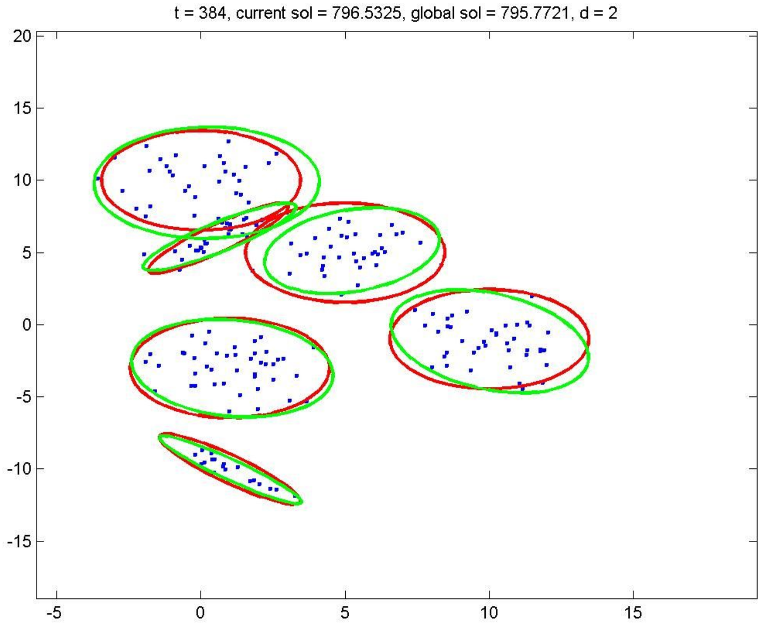
$$\phi_j = \frac{1}{N} \Sigma_{n=1}^{N} w_{n,j}$$

$$\mu_j = \frac{\Sigma_{n=1}^{N} w_{n,j} x_n}{\Sigma_{n=1}^{N} w_{n,j}}$$

$$\sigma_j^2 = \frac{\Sigma_{n=1}^{N} w_{n,j} (x_n - \mu_j)^2}{\Sigma_{n=1}^{N} w_{n,j}}$$

EM/GMM notes

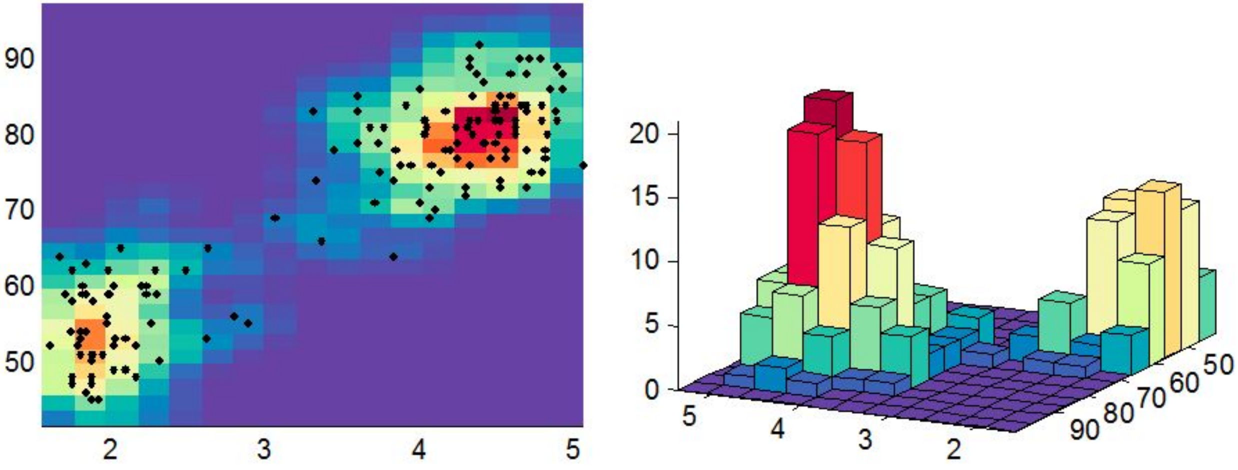
- Converges to local maxima (maximizing likelihood)
  - Just like k-means, need to try different initialization points
- What if it’s a multivariate Gaussian?
  - The grid search gets harder as the number of number of dimension grows



https://www.mathworks.com/matlabcentral/fileexchange/7055-multivariate-gaussian-mixture-model-optimization-by-cross-entropy

Histogram estimation in N-dimension

- Cut the space into N-dimensional cube
  - How many cubes are there?
  - Assume I want around 10 samples per cube to be able to estimate a nice distribution without overfitting. How many more samples do I need per one additional dimension?



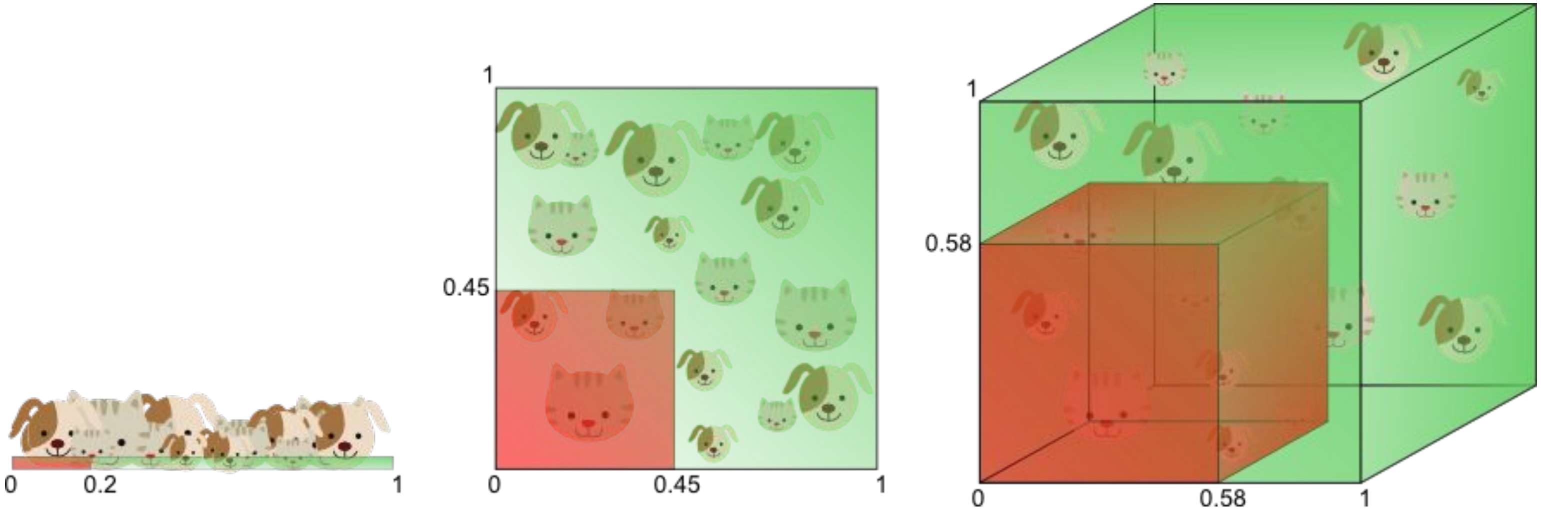
https://www.mathworks.com/matlabcentral/fileexchange/45325-efficient-2d-histogram--no-toolboxes-needed

The curse of dimensionality

https://erikbern.com/2015/10/20/nearest-neighbors-and-vector-models-epilogue-curse-of-dimensionality.html

The Curse of Dimensionality

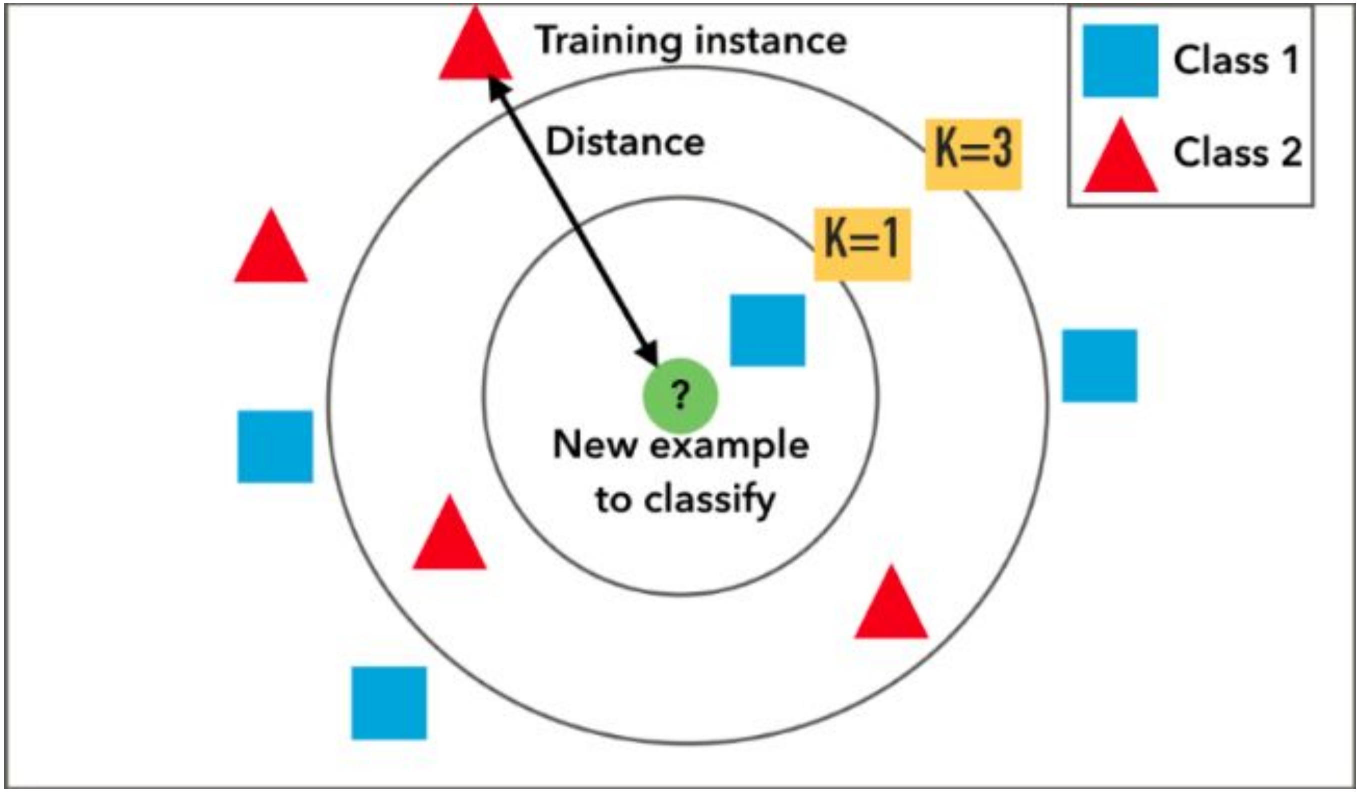
- Harder to visualize or see structure of
  - Verifying that data come from a straight line/plane needs n+1 data points
- Hard to search in high dimension – More runtime
- Need more data to get a get a good estimation of the data



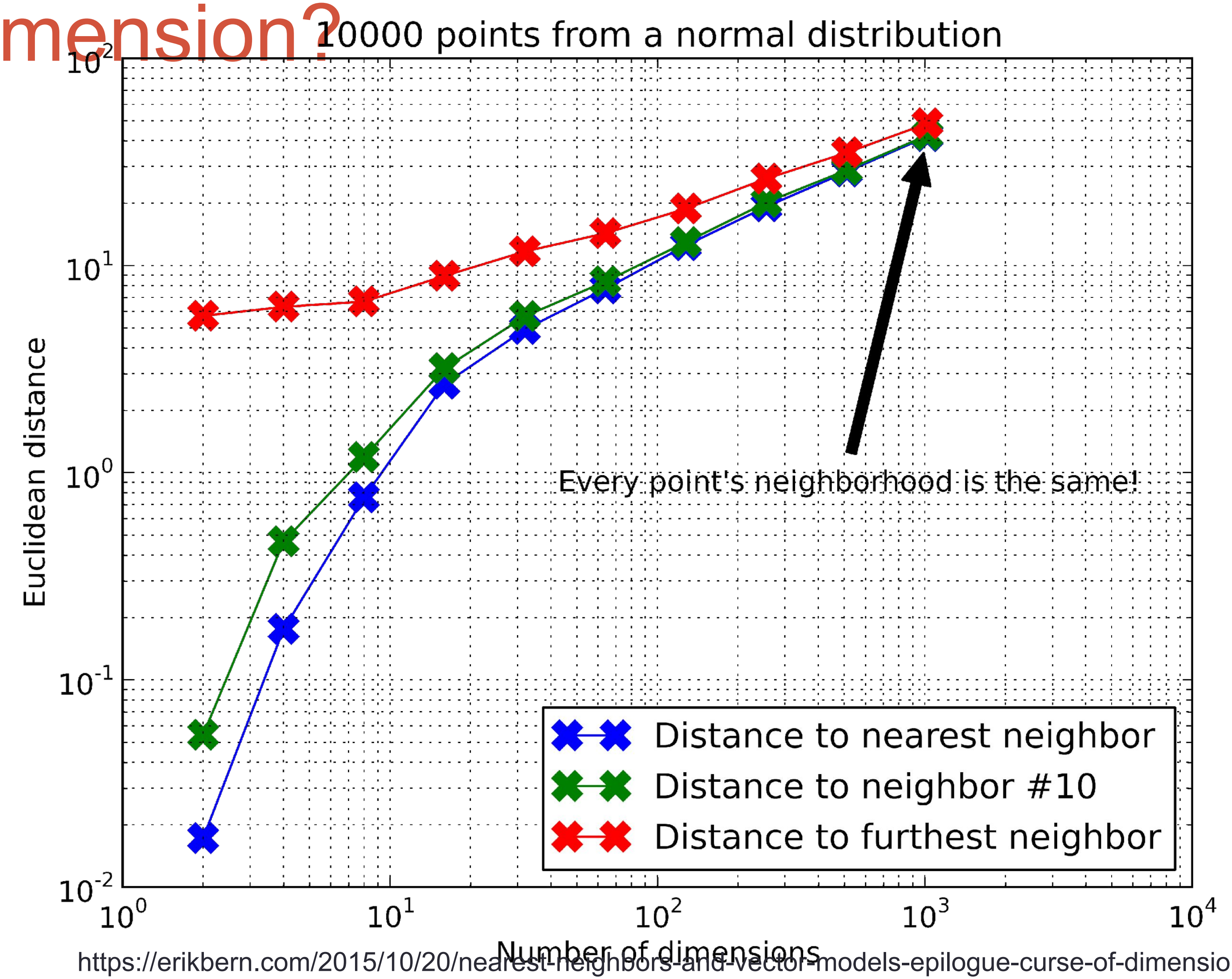
http://www.visiondummy.com/2014/04/curse-dimensionality-affect-classification/

K-Nearest Neighbor Classifier

- Nearest neighbor is susceptible to label noise
- Use the k-nearest neighbors as the classification decision
  - Use majority vote



What’s wrong with knn in high dimension?



https://erikbern.com/2015/10/20/nearest-neighbors-and-vector-models-epilogue-curse-of-dimensionality.html

Combating the curse of dimensionality

- Feature selection
  - Keep only “Good” features
- Feature transformation (Feature extraction)
  - Transform the original features into a smaller set of features

Feature selection vs Feature transform

- Keep original features
  - Useful for when the user wants to know which feature matters
    - But, correlation does not imply causation…

- New features (a combination of old features)
- Usually more powerful
  - Captures correlation between features

Feature selection

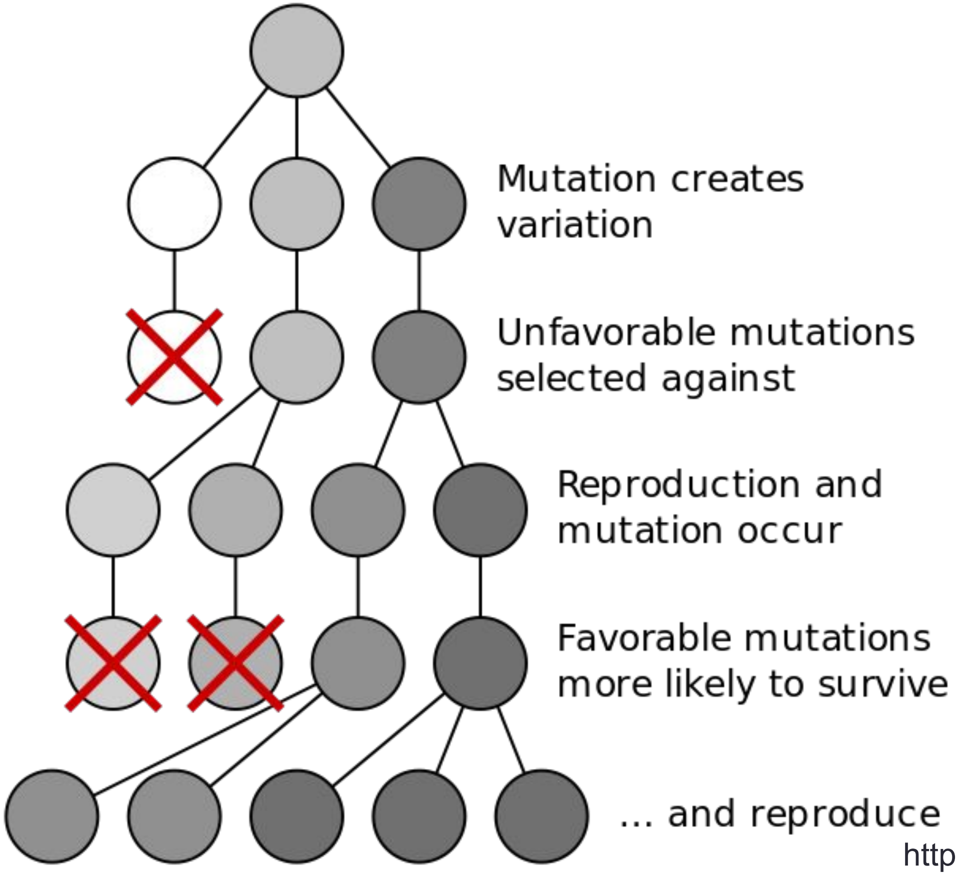
- Hackathon level (time limit days-a week)
  - Drop missing features
  - Low variance rows
    - A feature that is a constant is useless. Tricky in practice
  - Forward or backward feature elimination
    - Greedy algorithm: create a simple classifier with n-1 features, n times. Find which one has the best accuracy, drop that feature. Repeat.

Feature selection

- Proper methods
  - Algorithm that handles high dimension well and do selection as a by product
  - Tree-based classifiers
    - Random forest
  - Adaboost
  - Genetic Algorithm

Genetic Algorithm

- A method based inspired by natural selection
  - No theoretical guarantees but often work



Mutation creates variation

Unfavorable mutations selected against

Reproduction and mutation occur

Favorable mutations more likely to survive

... and reproduce

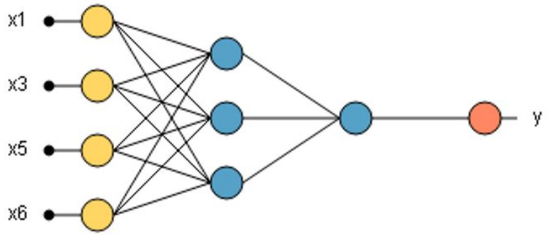
https://elitedatascience.com/dimensionality-reduction-algorithms

Genetic Algorithm

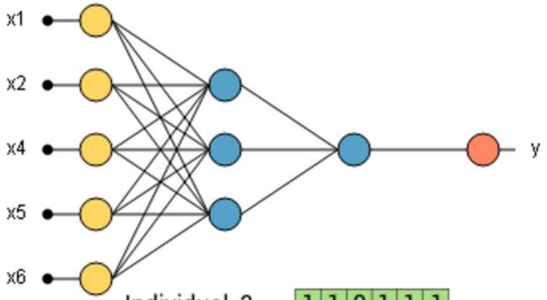
- Initialization
  - Create N classifiers, each using different subset of features
- Selection process
  - Rank the N classifiers according to some criterion, kill the lower half
- Crossover
  - The remaining classifier breeds offsprings by selecting traits from the parents
- Mutation
  - The offsprings can have mutations by random in order to generate diversity
- Repeat till satisfied

Initialization

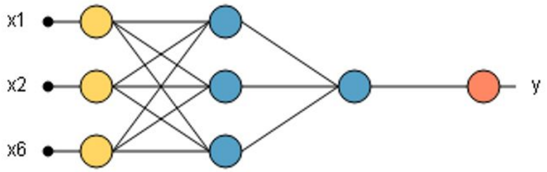
- Create N classifiers
- Randomly select a subset of features to use



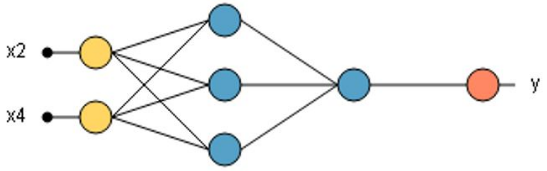
Individual 1 | 1 | 0 | 1 | 0 | 1 | 1 |



Individual 2 | 1 | 1 | 0 | 1 | 1 | 1 |



Individual 3 | 1 | 1 | 0 | 0 | 0 | 1 |

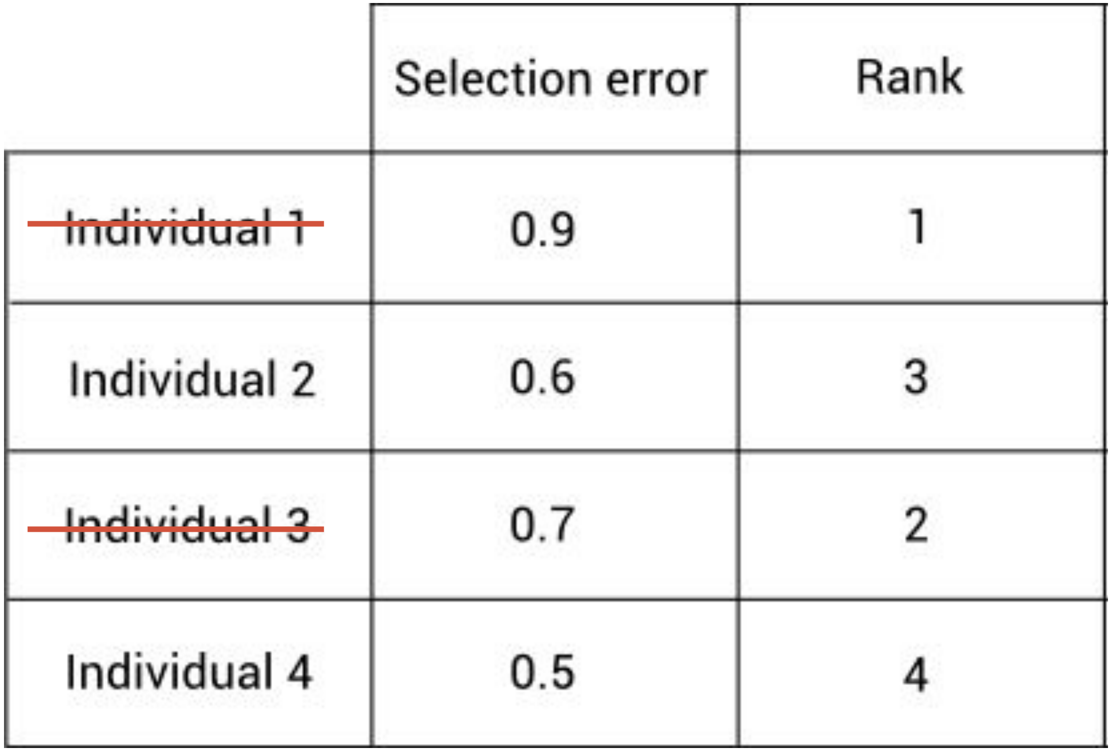


Individual 4 | 0 | 1 | 0 | 1 | 0 | 0 |

Examples from https://www.neuraldesigner.com/blog/genetic_algorithms_for_feature_selection

Selection process

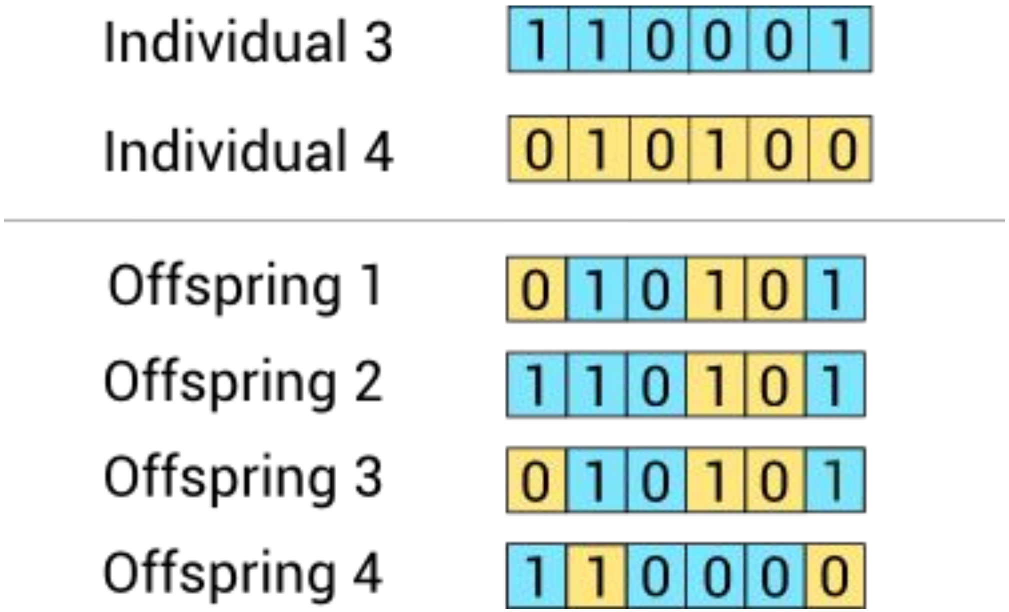
- Score the classifiers and kill the lower half (the amount to kill is also a parameter)



	Selection error	Rank
~~Individual 1~~	0.9	1
Individual 2	0.6	3
~~Individual 3~~	0.7	2
Individual 4	0.5	4

Crossover

- Breed offsprings by randomly select genes from parents



Individual 3 1 1 0 0 0 1

Individual 4 0 1 0 1 0 0

Offspring 1 0 1 0 1 0 1

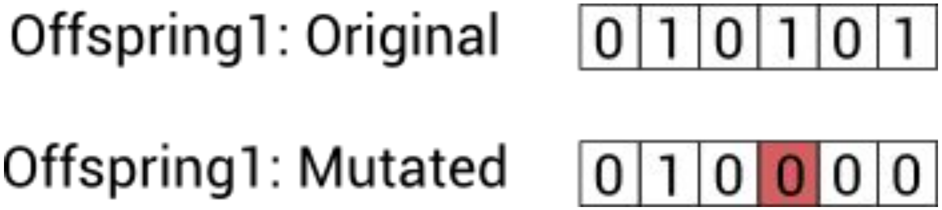
Offspring 2 1 1 0 1 0 1

Offspring 3 0 1 0 1 0 1

Offspring 4 1 1 0 0 0 0

Mutation

- Offspring can mutate with some probability to introduce diversity
- Mutation rate is usually 1/k where k is the number of features.
  - On average you mutate once per individual

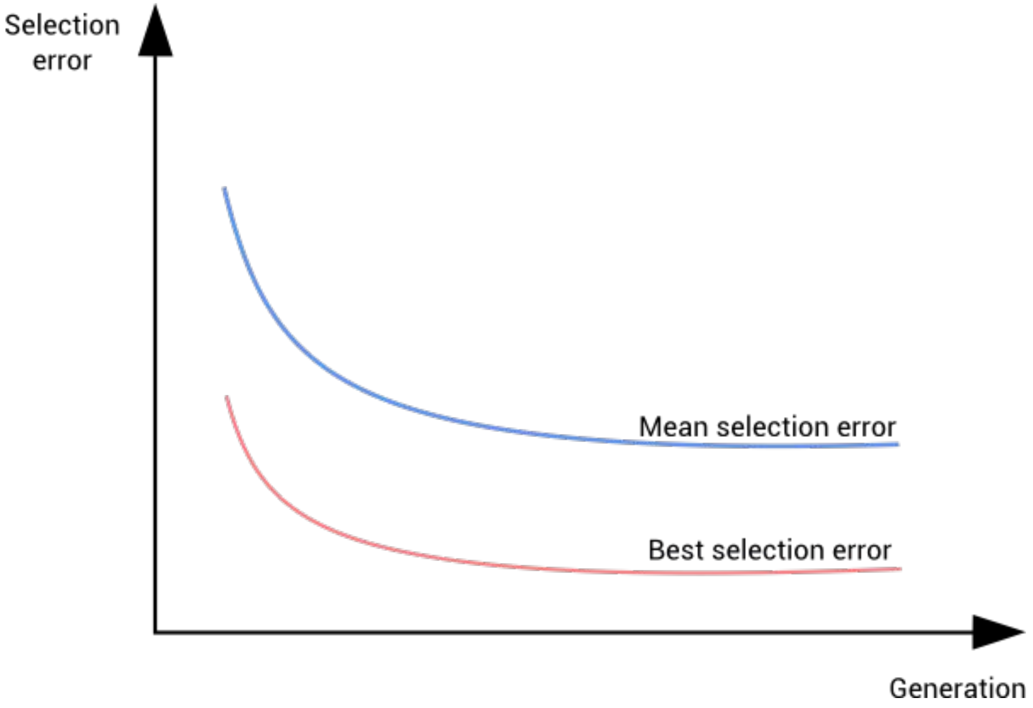


Offspring1: Original	0	1	0	1	0	1
Offspring1: Mutated	0	1	0	0	0	0

Performance

- Usually performs well. The general population usually gets better (mean). The best performing (individual) also gets better after each generation
- Can be use to tune neural networks!

https://blog.coast.ai/lets-evolve-a-neural-network-with-a-genetic-algorithm-code-included-8809bece164

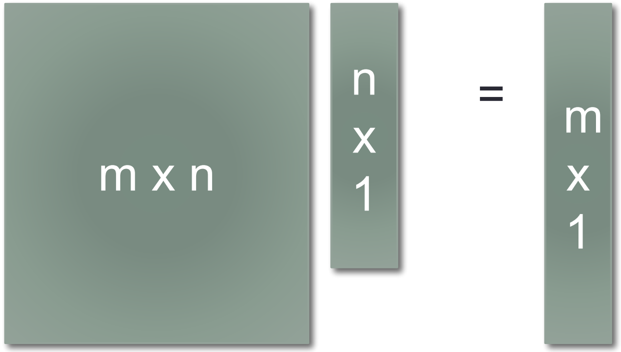


Feature transformation

- Principal Component Analysis
- Linear Discriminant Analysis (NOT Latent Dirichlet Allocation)
- Random Projections

Linear Algebra Review

- Think Sets and Functions, rather than manipulation of number arrays/rectangles



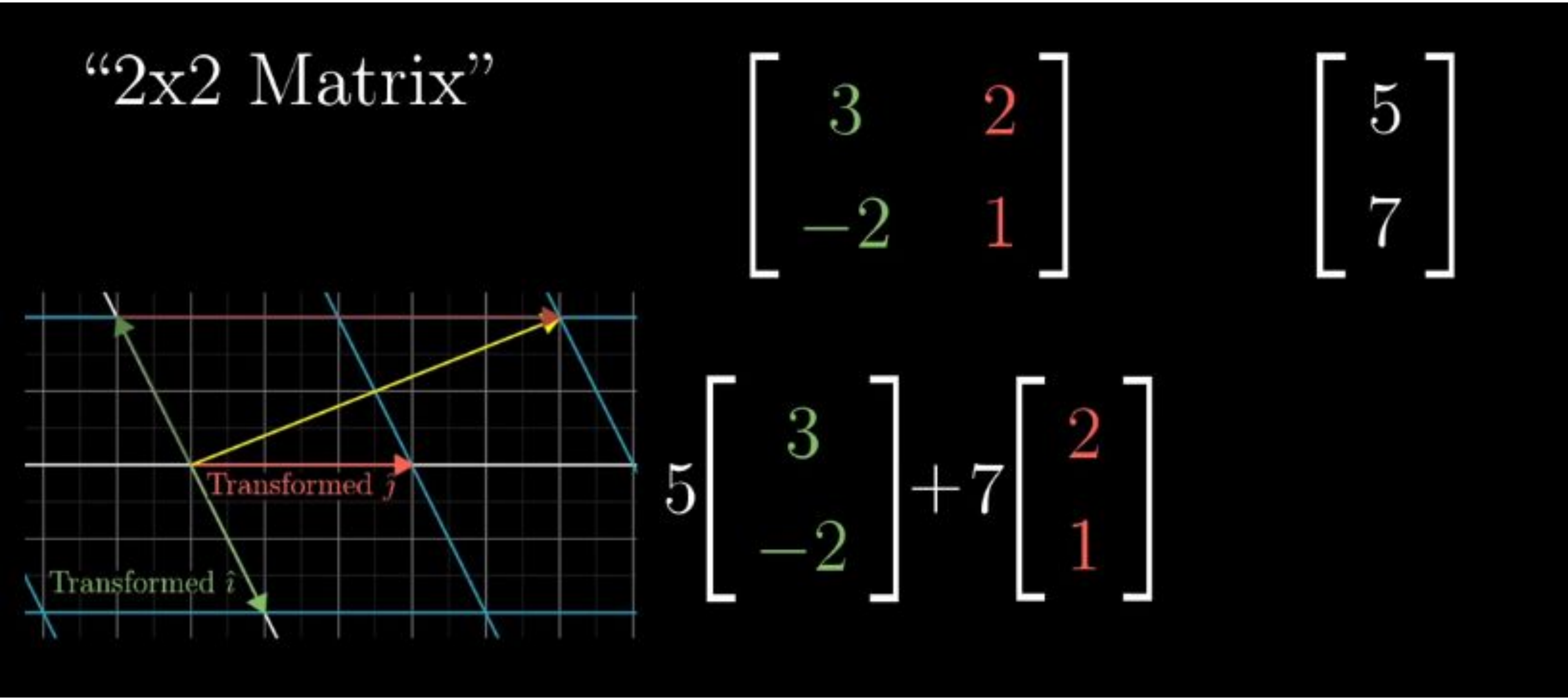
$f:R^n$ -> R^m

$f(\mathbf{x})$

https://www.linkedin.com/pulse/key-machine-learning-prereq-viewing-linear-algebra-through-ashwin-rao

Linear Algebra Review

- Matrix as a sequence of column vectors



“2x2 Matrix”

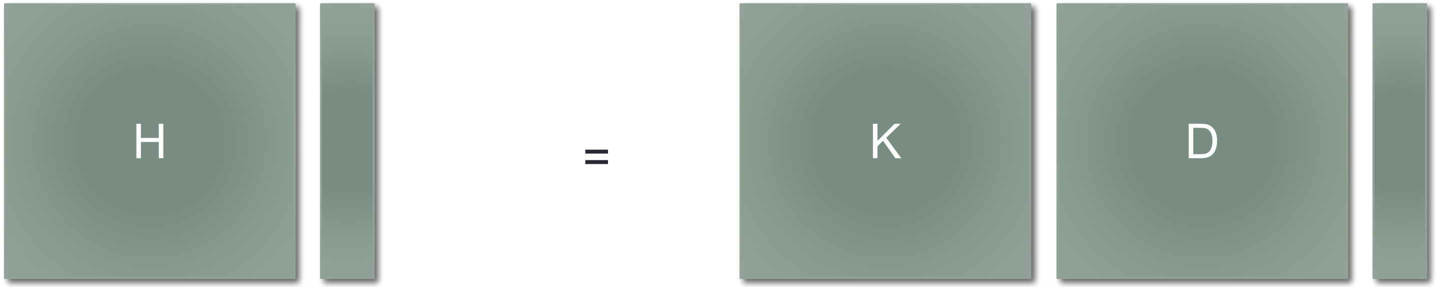
$$\begin{bmatrix} 3 & 2 \\ -2 & 1 \end{bmatrix} \qquad \begin{bmatrix} 5 \\ 7 \end{bmatrix}$$

$$5\begin{bmatrix} 3 \\ -2 \end{bmatrix} + 7\begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

https://www.youtube.com/watch?v=kYB8IZa5AuE&list=PLZHQObOWTQDPD3MizzM2xVFitgF8hE_ab&index=4

Linear Algebra Review

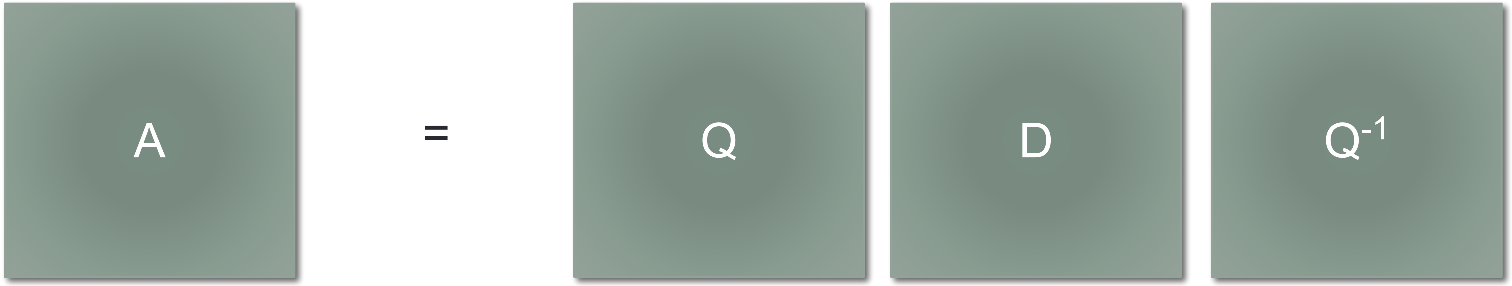
- Understand Matrix Factorizations as Compositions of “Simple” Functions:

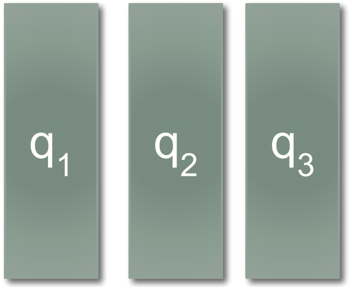


$$h(\mathbf{x}) \quad = \quad k(\, d(\mathbf{x})\,)$$

Linear Algebra Review

- View Eigendecomposition (ED) and Singular Value Decomposition (SVD) as rotations and stretches

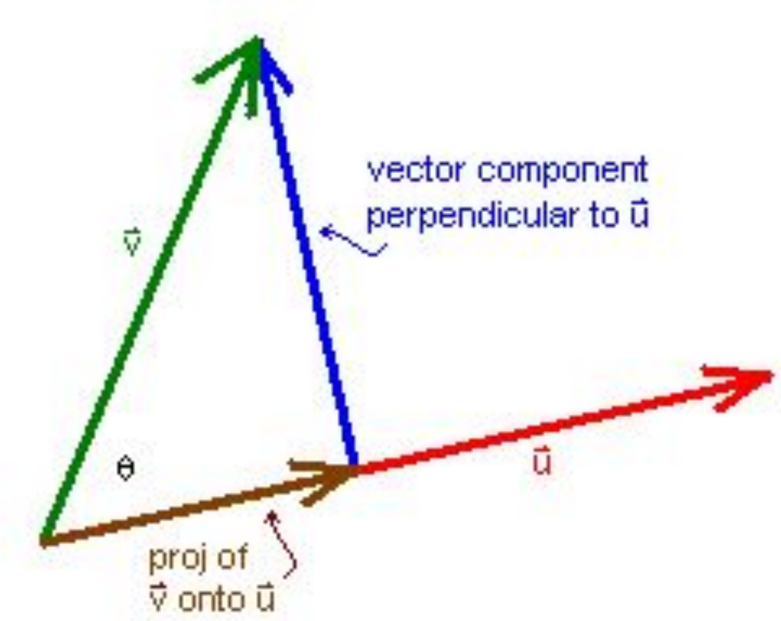




D has eigenvalues on the diagonal
Q is a matrix where ith column is the qth eigenvector

Linear Algebra Review

- Projection as a change of basis
- Change basis from x,y coordinates to be on u



$u^t v$

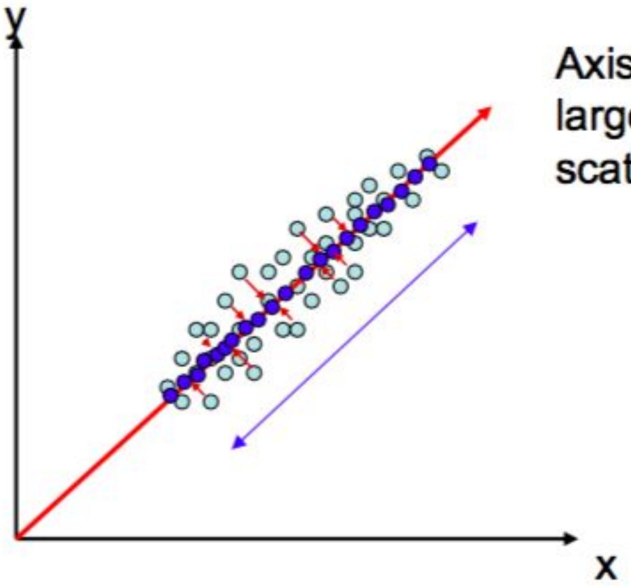
Positive semi-definite and eigen decomposition

- Covariance matrix is positive semi-definite and symmetric.
- Eigenvalues are nonnegative, eigenvalues and vectors are real values, eigenvectors are mutually orthogonal.

- $q_i^t q_j$ = 0 for i != j

What is PCA?

- We want to reduce the dimensionality but keep useful information
  - What is useful information? Variation
- We want to find a projection (a transformation) that describe maximum variation



Axis that describes the largest variation (or scatter)

PCA and LDA Slides from Marios Savvides

Formulation

- Maximize the variance after projection ie
  - argmax Var($\mathbf{w}^t$ $\mathbf{x}$)
- Subject to w is a unit vector

- $\Sigma\mathbf{w} = \lambda\mathbf{w}$ <- eigenvector

Trace properties

1 - tr (a) = a
2 - trA = trA^T
3 - tr(A+B) = trA+trB
4 - tr(aA) = atr(A)

5 $$\nabla_A trAB = B^T$$

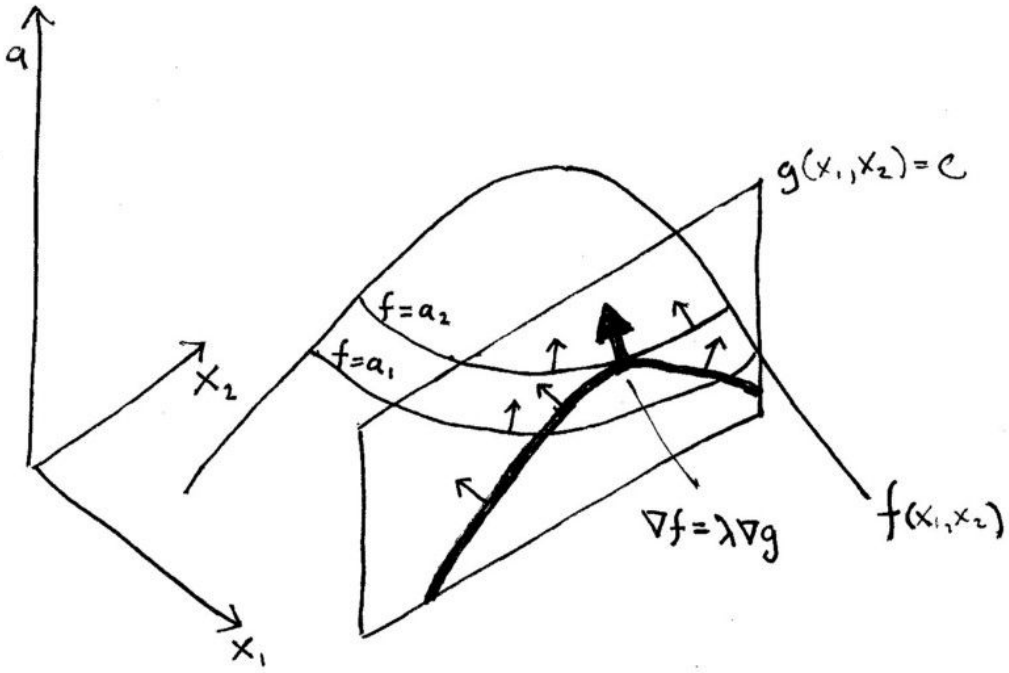
6 $$\nabla_{A^T} f(A) = (\nabla_A f(A))^T$$

7 $$\nabla_A trABA^TC = CAB + C^TAB^T$$

8 $$\nabla_{A^T} trABA^TC = B^TA^TC^T + BA^TC$$

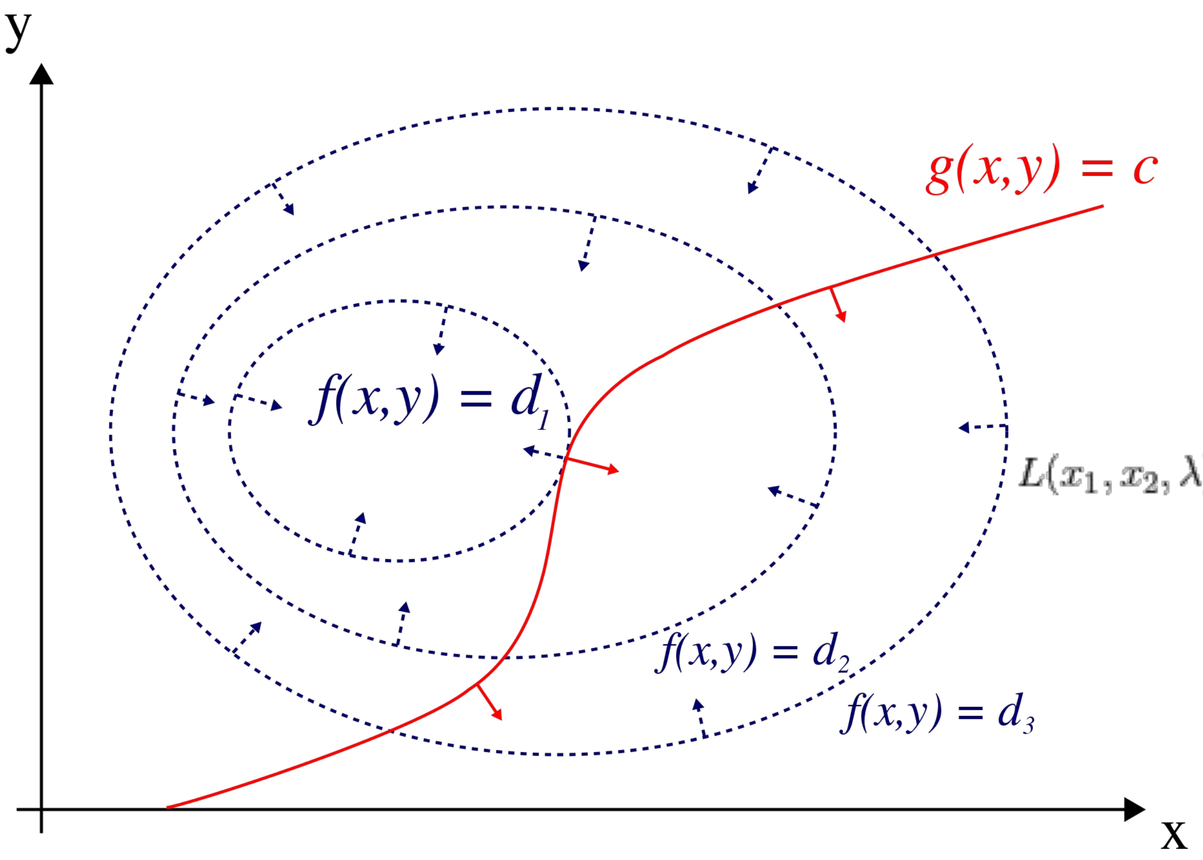
Lagrange Multiplier

https://medium.com/@andrew.chamberlain/a-simple-explanation-of-why-lagrange-multipliers-works-253e2cdcbf74



$$L(x_1,x_2,\lambda) = f(x_1,x_2) - \lambda(g(x_1,x_2) - c)$$

$$\nabla L = \begin{bmatrix} \frac{\partial f}{\partial x_1} - \lambda\frac{\partial g}{\partial x_1} \\ \frac{\partial f}{\partial x_2} - \lambda\frac{\partial g}{\partial x_2} \\ g(x_1,x_2) - c \end{bmatrix} = 0$$



$$L(x_1, x_2, \lambda) = f(x_1, x_2) - \lambda(g(x_1, x_2) - c)$$

$$\nabla L = \begin{bmatrix} \frac{\partial f}{\partial x_1} - \lambda \frac{\partial g}{\partial x_1} \\ \frac{\partial f}{\partial x_2} - \lambda \frac{\partial g}{\partial x_2} \\ g(x_1, x_2) - c \end{bmatrix} = 0$$

https://en.wikipedia.org/wiki/Lagrange_multiplier#/media/File:LagrangeMultipliers2D.svg

So we got to eigenvectors

- A dxd covariance matrix has d eigenvectors/values pair. Do we use all of them?
- Which pair to use?

Selecting eigenvectors

- Remember the variance of projected data is

$$\omega^T \Sigma \omega. \quad (1)$$

- And our solution yielded

$$\Sigma\omega = \lambda\omega \qquad (2)$$

- Plug (2) in (1) and we get

projected variance $= \omega^T \Sigma \omega = \omega^T \lambda\omega$

$= \lambda \omega^T \omega$ (remember $||\omega||=1$)

$= \lambda$

PCA

- The direction vector captures the variance corresponding to the eigenvalue
- So we want the higher eigenvalues
  - How many?

Matrix rank

- A square dxd matrix has full rank (e.g. rank d) if the columns are linearly independent.
- The number of linearly independent columns is the rank of the matrix

- A covariance matrix of size dxd will have have at most N-1 rank where N is the number of training samples
  - 640x640 images = ~400000 dimensions
  - 1000 training images
  - The covariance matrix will be at most rank 999. The missing rank is because of the mean.

PCA

- The direction vector captures the variance corresponding to the eigenvalue
- So we want the higher eigenvalues
- Take the eigenvalues with non-zero eigenvalues (at most N-1 non-zero eigenvalues)

Basis decomposition

- Let’s consider our projection w_i which is the eigenvectors to be a basis vector v_i
- We can represent any vector as a sum of basis vectors as follows:

$$\mathbf{x} = \sum_{i=1}^{N} p_i \mathbf{v}_i = p_1 \begin{bmatrix} | \\ \mathbf{v}_1 \\ | \end{bmatrix} + p_2 \begin{bmatrix} | \\ \mathbf{v}_2 \\ | \end{bmatrix} + .. + p_n \begin{bmatrix} | \\ \mathbf{v}_{n} \\ | \end{bmatrix} = \mathbf{V}\mathbf{p}$$

Finding the weights

$$\mathbf{x} = \sum_{i=1}^{N} p_i \mathbf{v}_i = p_1 \begin{bmatrix} | \\ \mathbf{v}_1 \\ | \end{bmatrix} + p_2 \begin{bmatrix} | \\ \mathbf{v}_2 \\ | \end{bmatrix} + .. + p_n \begin{bmatrix} | \\ \mathbf{v}_n \\ | \end{bmatrix} = \mathbf{V}\mathbf{p}$$

- If v_i are orthogonal, the projection of x onto v_i gives p_i

$$\mathbf{V}^{\mathrm{T}}\mathbf{x} = \begin{bmatrix} - & \mathbf{v}_1 & - \\ - & \mathbf{v}_2 & - \\ - & \mathbf{v}_3 & - \end{bmatrix} \begin{bmatrix} | \\ \mathbf{x} \\ | \end{bmatrix} = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

Means

- In PCA, we model variance. (Variation around the mean)
- In our projection we need to remove the mean

$$\mathbf{p} = \mathbf{V}^{\mathrm{T}}(\mathbf{x} - \mathbf{m})$$

- The mean is the mean of all your training data
- If we want to reconstruct the data we need to add back the mean

$$\mathbf{x} = \sum_{i=1}^{N} p_i \mathbf{v}_i + \mathbf{m} = p_1 \begin{bmatrix} | \\ \mathbf{v}_1 \\ | \end{bmatrix} + p_2 \begin{bmatrix} | \\ \mathbf{v}_2 \\ | \end{bmatrix} + .. + p_n \begin{bmatrix} | \\ \mathbf{v}_n \\ | \end{bmatrix} + \mathbf{m} = \mathbf{V}\mathbf{p} + \mathbf{m}$$

Practical issues

- If your data has different magnitudes in different dimensions, normalize each dimension before PCA

- If we have 640x640 images = ~400000 dimensions.
- What is the size of the covariance matrix?

Practical issues

- You have N training examples.
- For the case where N << 400000, we only have N-1 eigenvalues we care about anyway

Gram Matrix

$$\Sigma = E(x - \mu)(x - \mu)^T = XX^T$$

Covariance matrix is the outer-product of the input matrix

Must solve $\Sigma v = \lambda v$

$XX^T v = \lambda v$ (pre-mult by X^T) (1)

$X^T XX^T v = \lambda X^T v$ ($v' = X^T v$) (2)

Solve eigenvalue problem $X^T X v' = \lambda v'$

- $X^T X$ is a gram of inner-product matrix. Its size is NxN where N is the number of data samples.

But how to get v from v'?

- From previous slide, equation (1) and (2)
  - $XX^Tv = \lambda v$ (1)
  - $v' = X^Tv$ (2)
- Substitute (2) into (1)
  - $Xv' = \lambda v$

- Thus, $v = Xv'$. We don't care about the scaling term because we will always scale the eigenvector so that it is orthonormal i.e. $||v|| = 1$.

How many eigenvectors?

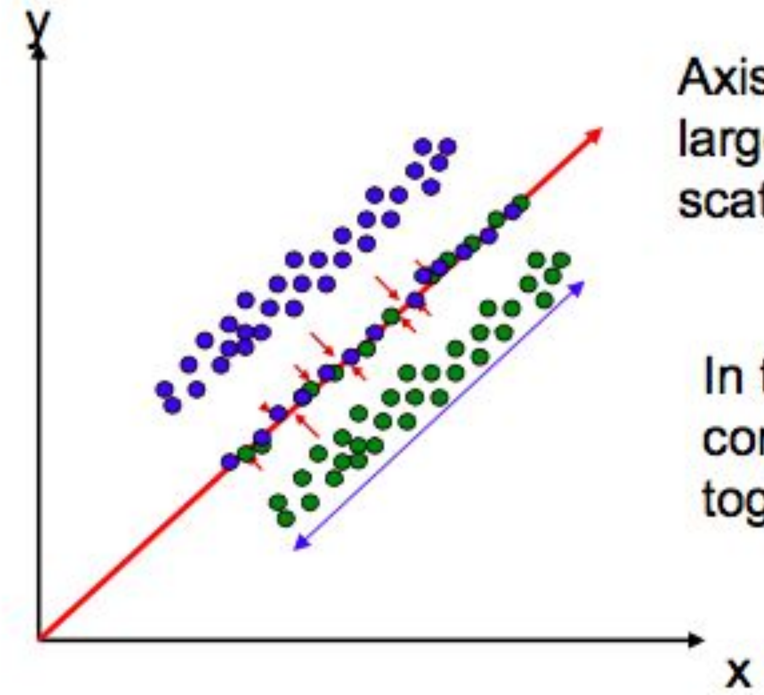
- Select based on amount of variance explained
  - Sum of eigenvalues exceeds some percent of total
- Reconstruction error

$$\mathbf{x} = \sum_{i=1}^{N} p_i \mathbf{v}_i = p_1 \begin{bmatrix} | \\ \mathbf{v}_1 \\ | \end{bmatrix} + p_2 \begin{bmatrix} | \\ \mathbf{v}_2 \\ | \end{bmatrix} + .. + p_n \begin{bmatrix} | \\ \mathbf{v}_n \\ | \end{bmatrix} = \mathbf{V}\mathbf{p}$$

  - Select enough v so that the difference between original x and reconstructed x is small

PCA for classification

- PCA does not cares about the class labels

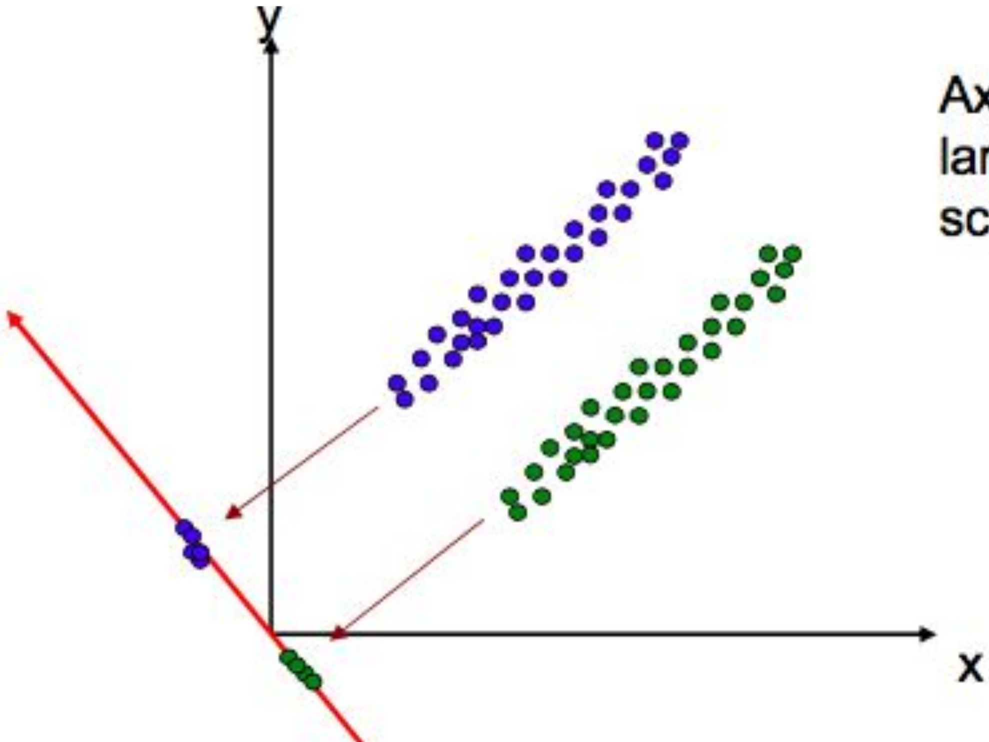


Axis that describes the largest variation (or scatter)…

In this case the projection vector completely smears the two classes together, making them in-separable

What is LDA

- Find the projections that separate the classes.
- Assumes unimodal Gaussian model for each class
    - Maximize the distance between the means and minimize the variance of each class -> best classification performance



Axis that describes the largest variation (or scatter)

Simple 2 class case

- We want to maximize the distance between the projected means:

e.g. maximize $|(\tilde{\mu}_1 - \tilde{\mu}_2)|^2$

Where $\tilde{\mu}_1$ is the projected mean $\boldsymbol{\mu}_1$ of class onto LDA direction vector **w** , i.e.

$$\tilde{\mu}_1 = \mathbf{w}^{\mathrm{T}}\boldsymbol{\mu}_1$$

and for class 2: $\tilde{\mu}_2 = \mathbf{w}^{\mathrm{T}}\boldsymbol{\mu}_2$ thus

$$|(\tilde{\mu}_1 - \tilde{\mu}_2)|^2 = |(\mathbf{w}^{\mathrm{T}}\boldsymbol{\mu}_1 - \mathbf{w}^{\mathrm{T}}\boldsymbol{\mu}_2)|^2$$

$$= \mathbf{w}^{\mathrm{T}}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^{\mathrm{T}}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^{\mathrm{T}}\mathbf{w}$$

$$= \mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathbf{B}}\mathbf{w}$$

Between class scatter matrix S_B

$$(\tilde{\mu}_1 - \tilde{\mu}_2)^2 = (\mathbf{w}^{\mathbf{T}}\boldsymbol{\mu}_1 - \mathbf{w}^{\mathbf{T}}\boldsymbol{\mu}_2)^2$$

$$= \mathbf{w}^{\mathbf{T}}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^{\mathbf{T}}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^{\mathbf{T}}\mathbf{w}$$

$$= \mathbf{w}^{\mathbf{T}}\mathbf{S}_{\mathbf{B}}\mathbf{w}$$

We want to maximize $w^T S_B w$ where S_B is the between class scatter matrix defined as:

$$\mathbf{S}_{\mathbf{B}} = (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^{\mathbf{T}}$$

We also want to minimize within class scatter

- The variance or scatter of each class. We also want to minimize them.

$$\tilde{s}_1^{\,2} = \sum_{i=1}^{N_1} (\tilde{x}_i - \tilde{\mu}_1)^2$$

Minimize the total scatter $\tilde{s}_1^{\,2} + \tilde{s}_2^{\,2}$

Within class scatter

- Lets expand on scatter s_1,s_2.

$$\tilde{s}_1^{\,2} = \sum_{i=1}^{N_1} (\tilde{x}_i - \tilde{\mu}_1)^2$$

$$= \sum_{i=1}^{N_1} (\mathbf{w}^{\mathrm{T}}\mathbf{x}_i - \mathbf{w}^{\mathrm{T}}\boldsymbol{\mu}_1)^2$$

$$= \sum_{i=1}^{N_1} \mathbf{w}^{\mathrm{T}}(\mathbf{x}_i - \boldsymbol{\mu}_1)(\mathbf{x}_i - \boldsymbol{\mu}_1)^{\mathrm{T}}\mathbf{w}$$

$$= \mathbf{w}^{\mathrm{T}}\mathbf{S}_1\mathbf{w}$$

Total within class scatter

- We want to minimize $\tilde{s}_1^2 + \tilde{s}_2^2$
- This is the same as $\mathbf{w}^T\mathbf{S}_w\mathbf{w}$

$$\mathbf{S}_{\mathbf{w}} = \sum_{i=1}^{C}\sum_{j=1}^{Ni} (\mathbf{x}_j - \boldsymbol{\mu}_i)(\mathbf{x}_j - \boldsymbol{\mu}_i)^{\mathrm{T}}$$

C number of classes, Ni number of images from class i

Fisher Linear Discriminant Criterion

- We want to maximize between class scatter
- We want to minimize within class scatter

- We have an objective function as a ratio so we can achieve both!

$$J(\mathbf{w}) = \frac{|(\tilde{\mu}_1 - \tilde{\mu}_2)|^2}{\tilde{s}_1{}^2 + \tilde{s}_2{}^2}$$

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S_B} \mathbf{w}}{\mathbf{w}^T \mathbf{S_W} \mathbf{w}}$$

LDA solution

- If you do calculus

$$\mathbf{S_B w} = \lambda \mathbf{S_W w}$$

$$\mathbf{S_W}^{-1}\mathbf{S_B w} = \lambda \mathbf{w}$$

If S_w is non-singular and invertible.

- Generalized eigenvalue problem. The number of solutions is min(rankS_B, rankS_W) = C-1 or N-C
- For 2 class this simplifies to
  - Note this is only one projection direction

$$\mathbf{w} = \mathbf{S_W}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$

LDA+PCA

- First do PCA to reduce dimension
- Then do LDA to maximize classification ability
- How many dimensions to PCA?
  - Do PCA to keep N-C eigenvectors -> Makes S_w full rank and invertible
  - Then, do LDA and compute C-1 projections in this N-C subspace
- PCA+LDA = Fisher projection

Random projection

- Original d-dimensional data is project to k-dimensional subspace
- Using a random k x d matrix R with unit norm columns
    - Johnson-Lindenstrauss lemma: If points in a vector space are projected onto a randomly selected subspace of suitably high dimension, then the distances between the points are approximately preserved

- Elements of R are usually selected from Gaussians.
    - Generally any zero mean unit variance distribution would satisfy Johnson-Lindenstrauss lemma.

Random projection notes

- R is not generally orthogonal.
  - But in a substantially large subspace, random vectors might be close to orthogonal.
- Looks weird but works…

Visualization

Methods covered

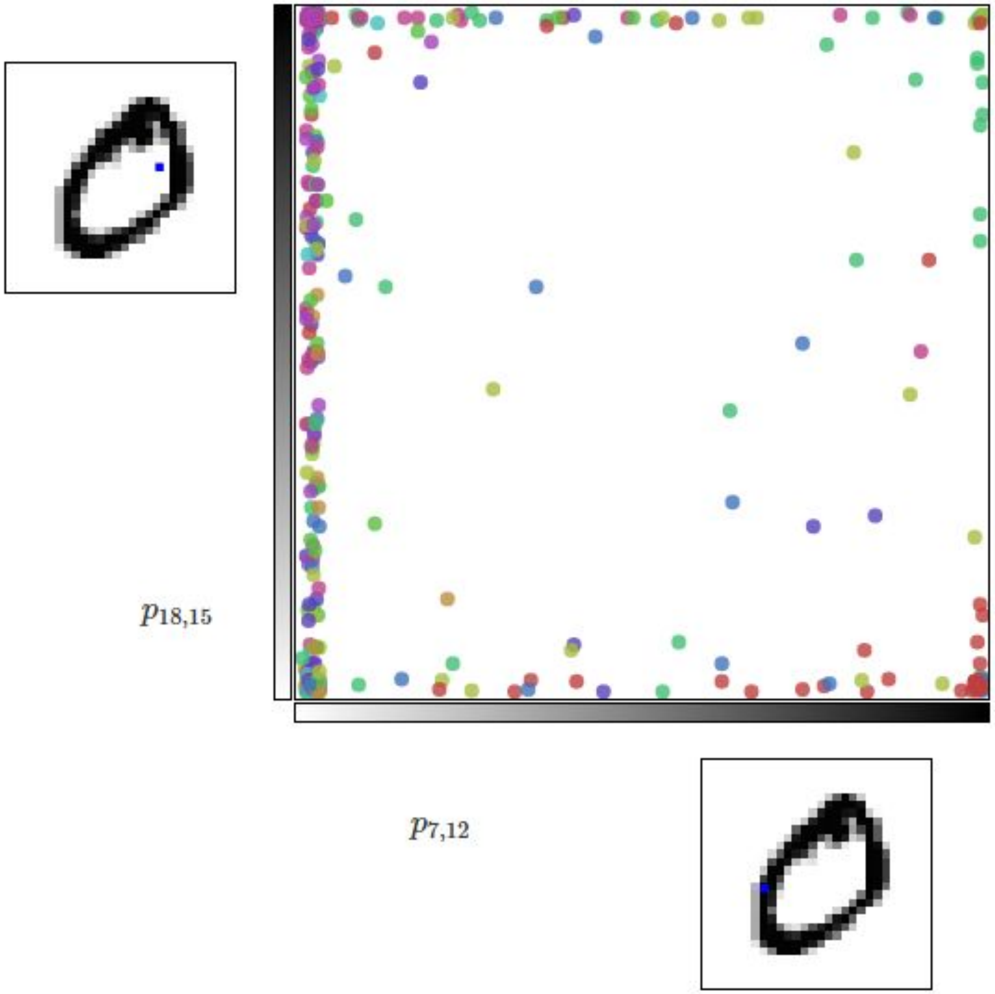
1. Reducing reconstruction error: PCA
2. Keeping direction of maximum separability: LDA
3. Preserving distance (globally): RP

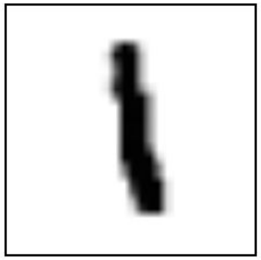
These are usually useful for downstream machine learning methods. (Classification/Regression/Clustering)

But what if we, as humans, want to get a sense of our data?

1. Interpretability (in some sense): ????

Visualizing MNIST

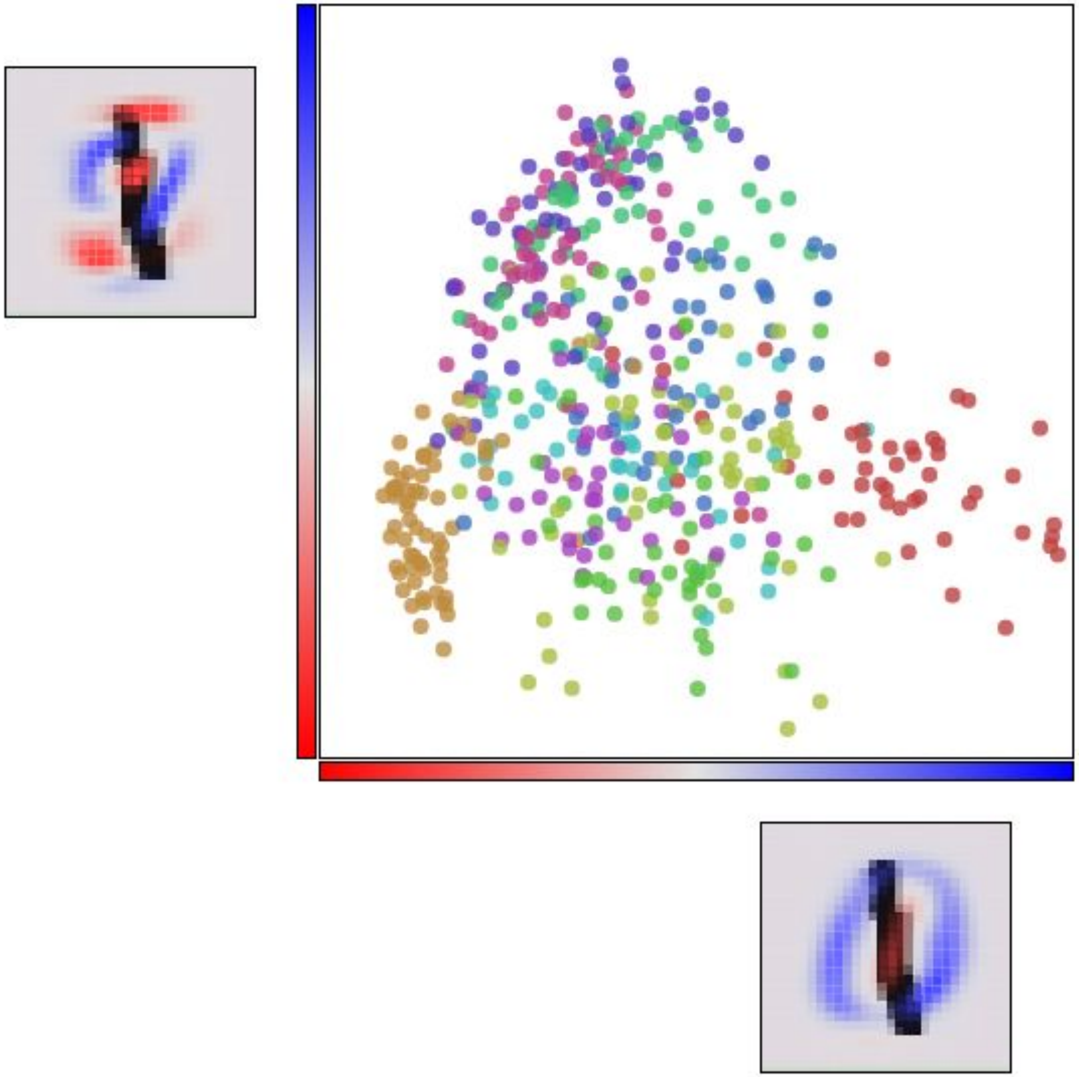


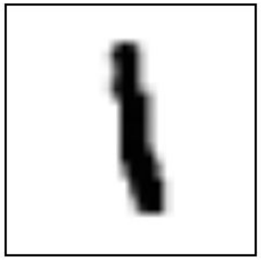


$$\cong \begin{bmatrix}
0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&.6&.8&0&0&0&0&0&0\\
0&0&0&0&0&0&.7&1&0&0&0&0&0&0\\
0&0&0&0&0&0&.7&1&0&0&0&0&0&0\\
0&0&0&0&0&0&.5&1&.4&0&0&0&0&0\\
0&0&0&0&0&0&0&1&.4&0&0&0&0&0\\
0&0&0&0&0&0&0&1&.4&0&0&0&0&0\\
0&0&0&0&0&0&0&1&.7&0&0&0&0&0\\
0&0&0&0&0&0&0&1&1&0&0&0&0&0\\
0&0&0&0&0&0&0&.9&1&.1&0&0&0&0\\
0&0&0&0&0&0&0&.3&1&.1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix}$$

http://colah.github.io/posts/2014-10-Visualizing-MNIST/

PCA with MNIST





$$\approx \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & .6 & .8 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & .7 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & .7 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & .5 & 1 & .4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & .4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & .4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & .7 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & .9 & 1 & .1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & .3 & 1 & .1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

http://colah.github.io/posts/2014-10-Visualizing-MNIST/

t-distributed Stochastic Neighbor Embedding (t-SNE)

Preserves neighbor (preserves local distance).

- Things close together should be close together in the projected space
- Prefer using few projected dimensions (2-3)

Defining neighbors

Define $P_{j|i}$ probability that *i* would pick *j* as its neighbor

Assume *i* picks proportional to Gaussian centered at *i*

$$p_{j|i} = \frac{exp(-||x_i - x_j||^2)/2\sigma_i^2}{\sum_{k \neq i} exp(-||x_i - x_k||^2)/2\sigma_i^2}$$

$P_{i|i}$ = 0 since we don't want to have it pick itself

The variance is fixed to some value.

Defining neighbors

Define $q_{j|i}$ probability that *i* would pick *j* as its neighbor

Assume *i* picks proportional to Gaussian centered at *i*

$$p_{j|i} = \frac{exp(-||x_i - x_j||^2)/2\sigma_i^2}{\sum_{k \neq i} exp(-||x_i - x_k||^2)/2\sigma_i^2}$$

When projected to set of points $\{y_i\}$, define $q_{j|i}$ the probability that *i* would pick *j* in embedding/latent space

$$q_{j|i} = \frac{exp(-||y_i - y_j||^2)}{\sum_{k \neq i} exp(-||y_i - y_k||^2)}$$

We set the variance in the y space to be 1/sqrt(2)

Defining neighbors

$$p_{j|i} = \frac{exp(-||x_i - x_j||^2)/2\sigma_i^2}{\sum_{k \neq i} exp(-||x_i - x_k||^2)/2\sigma_i^2}$$

$$q_{j|i} = \frac{exp(-||y_i - y_j||^2)}{\sum_{k \neq i} exp(-||y_i - y_k||^2)}$$

We expect p and q to be the same -> small distance

How to measure distance between probability functions?

Kullback-Leibler (KL) divergence

KL divergence

Distance between two distributions

$$D_{KL}(P||Q) = \sum_i P(i) log \frac{P(i)}{Q(i)} = -\sum_i P(i) log \frac{Q(i)}{P(i)}$$

Note $D_{KL}(P||Q) \neq D_{KL}(Q||P)$ (Not a real distance)

Always positive. Equals 0 iff Q = P at every point.

P(head) = 0.5 P(tail) = 0.5

Q(head) = 0.7 Q(tail) = 0.3

$D_{KL}(P||Q)$ = 0.5*ln 0.5/0.7 + 0.5*ln 0.5/0.3 = 0.087

$D_{KL}(Q||P)$ = 0.7*ln 0.7/0.5 + 0.3*ln 0.3/0.5 = 0.082

Loss function

$$p_{j|i} = \frac{exp(-||x_i - x_j||^2)/2\sigma_i^2}{\sum_{k \neq i} exp(-||x_i - x_k||^2)/2\sigma_i^2} \qquad q_{j|i} = \frac{exp(-||y_i - y_j||^2)}{\sum_{k \neq i} exp(-||y_i - y_k||^2)}$$

We expect p and q to be the same -> small distance

Loss function

All points i

KL computes over j

$$\sum_i D_{KL}(p_i||q_i)$$

$$D_{KL}(P||Q) = \sum_i \boxed{P(j)} log \frac{P(i)}{Q(j)}$$

Note P can be considered as the weight for the distance

Where p is large but q is small -> large penalty

q is small but p is large -> small penalty

D(p||q) focuses on local structure in p

What are we minimizing wrt?

How to minimize loss?

From SNE to t-SNE

Symmetric density

t-distributed

Symmetric with joint probability

$$D_{KL}(P||Q) = \sum_i P(i) log \frac{P(i)}{Q(i)}$$

$p_{j|i} \neq p_{i|j}$

A point i far away from everything will have small $p_{j|i}$

- Location of points in q no longer matter

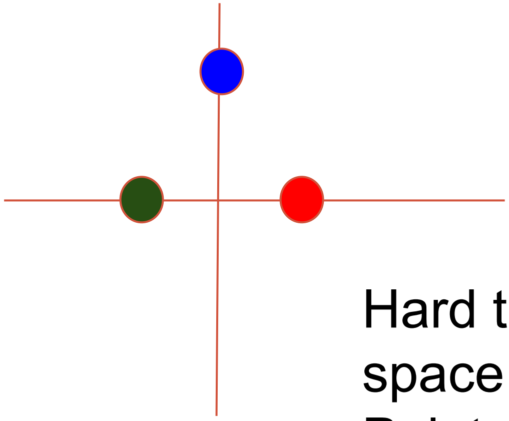
Create “joint probability” $p_{ij} = p_{ji} = (p_{i|j} + p_{j|i})/2$

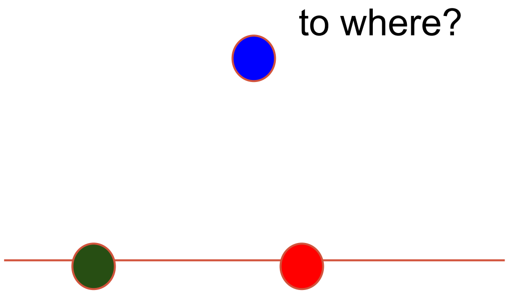
- Each data point will contribute to the loss

Use instead of conditional probability in KL divergence

t-distributed

- “Crowding problem”
- In N dimension, you can have N+1 points at equal distance. But you cannot model this in smaller dimension





Hard to cram information to a smaller dimension space

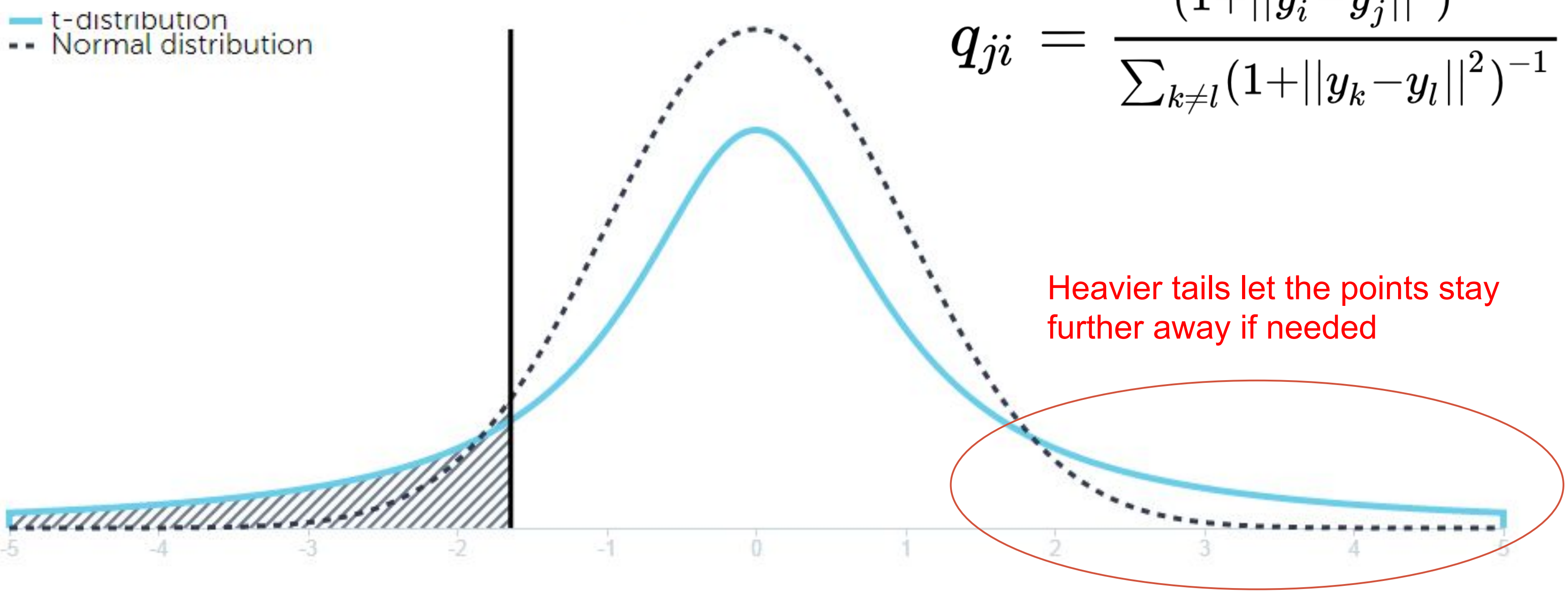
Points tend to cram in the embedding space (no gap)

t-distributed

- Instead of Gaussian for q we use student's t distribution

$$q_{ji} \propto (1 + ||y_i - y_j||^2)^{-1}$$

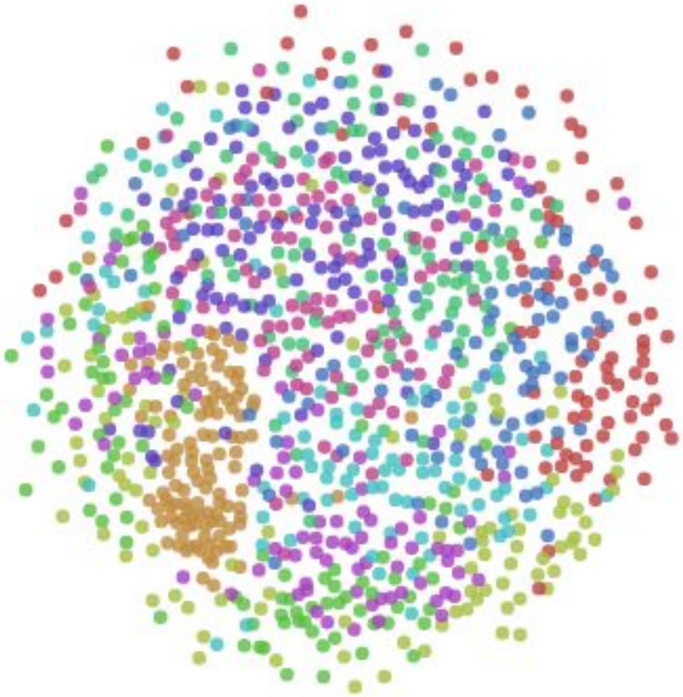
$$q_{ji} = \frac{(1+||y_i - y_j||^2)^{-1}}{\sum_{k \neq l}(1+||y_k - y_l||^2)^{-1}}$$



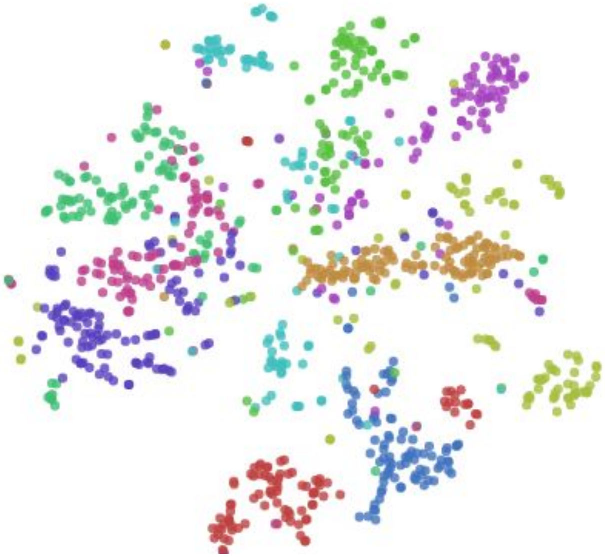
Heavier tails let the points stay further away if needed

http://rpsychologist.com/d3/tdist/

Crowding and t-SNE



Sammon's mapping
(crowding problem)



t-SNE

http://colah.github.io/posts/2014-10-Visualizing-MNIST/

Variance

$$p_{j|i} = \frac{exp(-||x_i - x_j||^2)/2\sigma_i^2}{\sum_{k \neq i} exp(-||x_i - x_k||^2)/2\sigma_i^2}$$

How to set the variance of our original space?

A single variance for all points is not ideal.

- Want small variance for dense parts
- Want big variance for sparse parts

Set variance by amount of neighbors you want!

How to quantify amount of neighbors?

Perplexity

$$p_{j|i} = \frac{exp(-||x_i - x_j||^2)/2\sigma_i^2}{\sum_{k \neq i} exp(-||x_i - x_k||^2)/2\sigma_i^2}$$

$$Perp(P_i) = 2^{H(P_i)}$$

$$H(P_i) = -\sum_j p_{j|i} log_2 p_{j|i}$$ Entropy

Perplexity of P_i represents effective amount of neighbors for the point i

Set Perp(P_i) then t-SNE algorithm searches for the corresponding variance

Typical values for perplexity 5 to 50

t-SNE summary

Goal: preserves local neighbors

Gradient-based -> need multiple runs to see the best

Two parameters: #iteration, perplexity

Does not learn a projection (unlike PCA, LDA, RP)

- If you have a new sample, you have to re-run the whole thing
- Might use a non-linear model to create learn t-SNE embeddings (deep learning)

Summary

- PCA
- LDA
  - PCA+LDA
- Random projection
- tSNE
- Homework

- Next time SVM