CPSC 340: Machine Learning and Data Mining

Sparse Matrix Factorization

Fall 2016

Admin

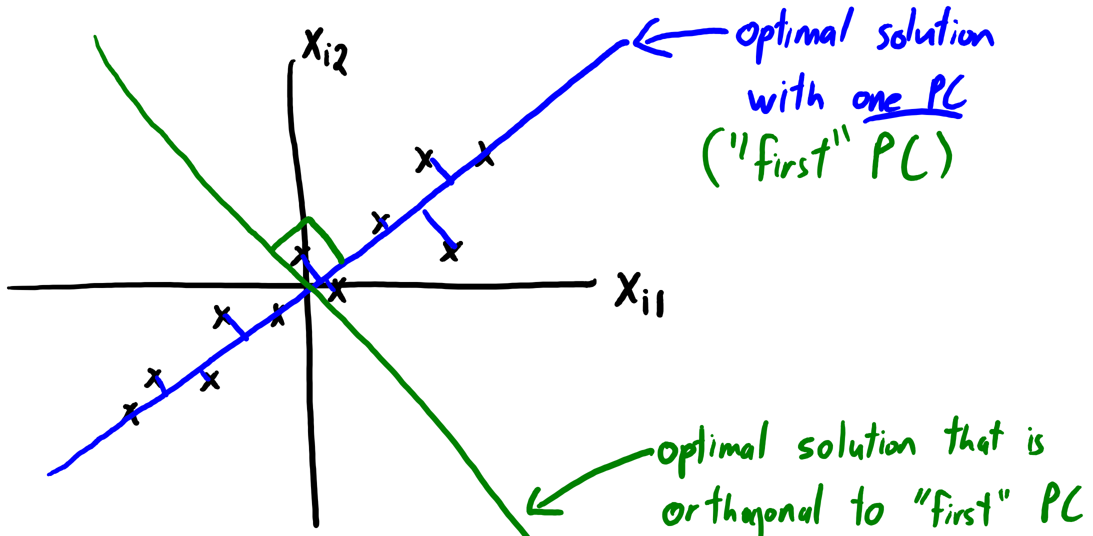
- Midterms:
  - Midterms can be viewed during office hours.
- Assignment 4:
  - Due Monday.
- Office hours:
  - Tuesday 2pm office hours moved to ICICS 104.
  - Extra office hours Thursdays from 4:30-5:30 in ICICS X836.
- Assignment 5:
  - Out on the weekend.

Last Time: PCA with Orthogonal/Sequential Basis

- When k = 1, PCA has a scaling problem.
- When k > 1, have scaling, orthogonality, rotation, label switching.
  - Standard fix: use normalized orthogonal rows w_c of 'W'.

$$w_c^T w_c = 1 \quad \text{and} \quad w_c^T w_{c'} = 0 \text{ for } c \neq c'$$

  - And fit the rows in order:
    - First row "explains the most variance" or "reduces error the most".



Last Time: Learning a Basis for Faces

- We discussed three ways to learn a basis z_i for faces:
  - K-means (vector quantization).
    - Replace face by the average face in a cluster.
    - Can’t distinguish between people in the same cluster (only ‘k’ possible faces).

$$x_i = z_{i1} * w_1 + z_{i2} * w_2 + z_{i3} * w_3 + z_{i4} * w_4 + z_{i5} * w_5 + z_{i6} * w_6$$

Last Time: Learning a Basis for Faces

- We discussed three ways to learn a basis z_i for faces:
  - K-means (vector quantization).
  - PCA (orthogonal basis).
    - Global average plus linear combination of "eigenfaces".
    - Can generate an infinite number of faces when changing the z_i.
    - But "eigenfaces" are not intuitive ingredients for faces.

Last Time: Learning a Basis for Faces

- We discussed three ways to learn a basis z_i for faces:
  - K-means (vector quantization).
  - PCA (orthogonal basis).
  - NMF (non-negative matrix factorization):
    - Instead of requiring orthogonality requires non-negativity.
      - No “ordering” among parts.
      - The z_i are sparse so each face only uses a subset of the sparse “parts”.

$$x_i = \mu + z_{i1} * w_1 + z_{i2} * w_2 + z_{i3} * w_3 + z_{i4} * w_4 + z_{i5} * w_5$$

Warm-up to NMF: Non-Negative Least Squares

- Consider our usual least squares problem:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w^Tx_i - y_i)^2$$

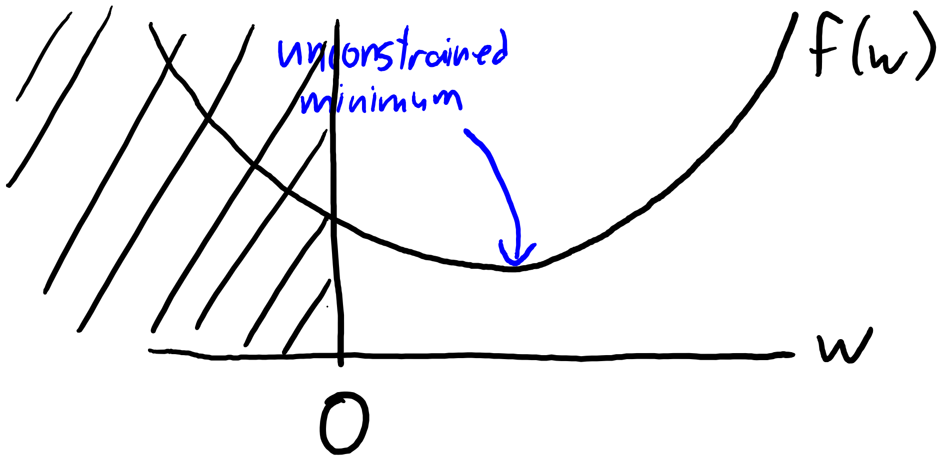
- But assume y_i and elements of x_i are non-negative:
  – Could be sizes (‘height’, ‘milk’, ‘km’) or counts (‘vicodin’, ‘likes’, ‘retweets’).
- Assume we want elements of ‘w’ to be non-negative, too:
  – No physical interpretation to negative weights.
  – If x_{ij} is amount of product you produce, what does $w_j < 0$ mean?
- Non-negativity tends to generate sparse solutions.

Sparsity and Non-Negative Least Squares

- Consider 1D non-negative least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w x_i - y_i)^2 \quad \text{with} \quad w > 0$$

- Plotting the (constrained) objective function:



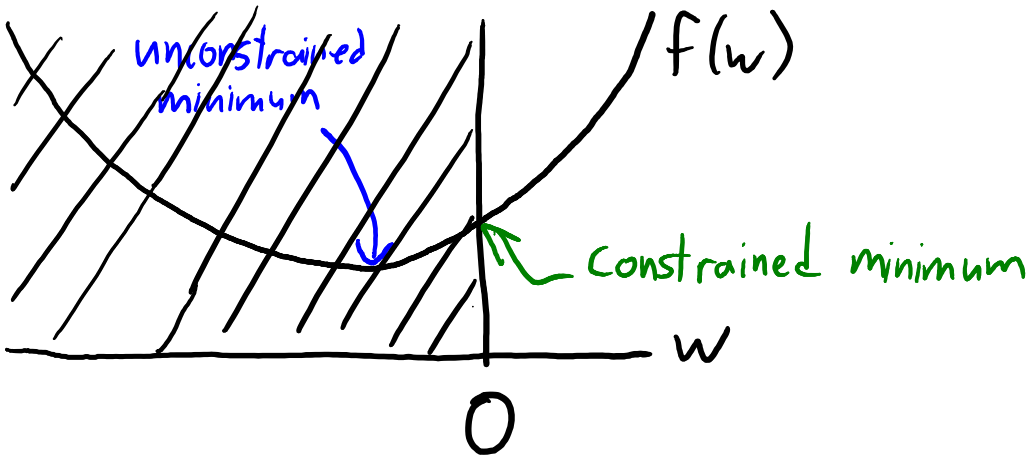
- In this case, non-negative solution is least squares solution.

Sparsity and Non-Negative Least Squares

- Consider 1D non-negative least squares objective:

$$f(w) = \frac{1}{2}\sum_{i=1}^{n}(w\,x_i - y_i)^2 \quad \text{with} \quad w \geq 0$$

- Plotting the (constrained) objective function:



- In this case, non-negative solution is w = 0.

Sparsity and Non-Negativity

- So non-negativity leads to sparsity.
  - Also regularizes: w_j are smaller since can't "cancel" out negative values.
- How can we minimize f(w) with non-negative constraints?
  - Naive approach: solve least squares problem, set negative w_j to 0.

    Compute $w = (X^T X) \backslash (X^T y)$

    Set $w_j = \max\{0, w_j\}$
  - This is correct when d = 1.
  - Can be worse than setting w = 0 when d ≥ 2.

Sparsity and Non-Negativity

- So non-negativity leads to sparsity.
  - Also regularizes: w_j are smaller since can't "cancel" out negative values.
- How can we minimize f(w) with non-negative constraints?
  - A correct approach is projected gradient algorithm:
    - Run a gradient descent iteration:

$$w^{t+1/2} = w^t - \alpha^t \nabla f(w^t)$$

    - After each step, set negative values to 0.

$$w_j^{t+1} = \max\{0, w_j^{t+1/2}\}$$

    - Repeat.

Sparsity and Non-Negativity

- Similar to L1-regularization, non-negativity leads to sparsity.
  - Also regularizes: w_j are smaller since can't "cancel" out negative values.
- How can we minimize f(w) with non-negative constraints?
  - Correct approach is "projected" gradient descent:

$$w^{t+1/2} = w^t - \alpha^t \nabla f(w^t) \qquad w_j^{t+1} = \max\{0, w_j^{t+1/2}\}$$

  - Similar properties to gradient descent:
    - Guaranteed decrease of 'f' if α_t is small enough.
    - Reaches local minimum under weak assumptions (global minimum for convex 'f').
    - Generalizations allow things like L1-regularization instead of non-negativity.

(findMinL1.m)

Projected-Gradient for NMF

- Back to the non-negative matrix factorization (NMF) objective:

$$f(W,Z) = \sum_{i=1}^{n}\sum_{j=1}^{d}(w_j^T z_i - x_{ij})^2 \quad \text{with } w_{cj} \geq 0 \text{ and } z_{ij} \geq 0$$

  – Different ways to use projected gradient:
    - Alternate between projected gradient steps on 'W' and on 'Z'.
    - Or run projected gradient on both at once.
    - Or sample a random 'i' and 'j' and do stochastic projected gradient.

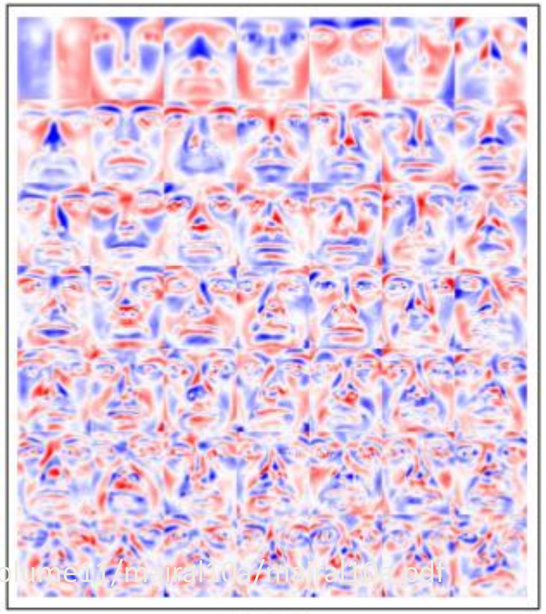
$$\text{Set } z_i^{t+1} = z_i^t - \alpha^t \nabla_{z_i} f(W,Z) \text{ and } w_j^{t+1} = w_j^t - \alpha^t \nabla_{w_j} f(W,Z) \text{ for } \underline{\text{selected}} \text{ } i \text{ and } j$$

(keep other values of W and Z fixed)

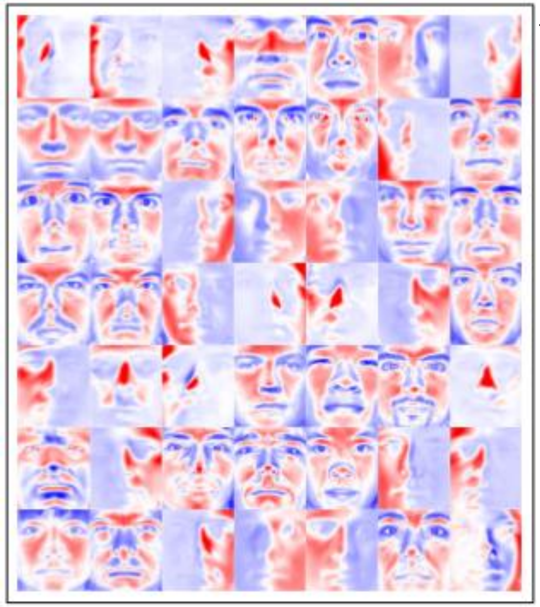
  – Non-convex and (unlike PCA) is sensitive to initialization.
    - Hard to find the global optimum.
    - Typically use random initialization.

Regularized Matrix Factorization

- For many PCA applications, ordering orthogonal PCs makes sense.
  - Latent factors are independent of each other.
  - We definitely want this for visualization.
- In other cases, ordering orthogonal PCs doesn't make sense.
  - We might not expect a natural "ordering".



Usual orthogonal eigenfaces



PCA with non-orthogonal basis

http://www.jmlr.org/papers/volume11/mairal10a/mairal10a.pdf

Regularized Matrix Factorization

- More recently people have considered L2-regularized PCA:

$$f(W,Z) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda_1}{2}\underbrace{\|W\|_F^2}_{\sum_{c=1}^{k}\sum_{j=1}^{d} w_{cj}^2} + \frac{\lambda_2}{2}\|Z\|_F^2$$

  - Replaces normalization/orthogonality/sequential-fitting.
    - But requires regularization parameters λ_1 and λ_2.
  - Need to regularize W and Z because of scaling problem:
    - Regularizing only 'W' won't work: you could make 'Z' big to compensate.
    - You could alternately constrain one and regularize the other:

$$f(W) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda}{2}\|Z\|_F^2 \quad \text{with } \|w_c\| \le 1 \text{ for all 'c'}$$

Sparse Matrix Factorization

- Instead of non-negativity, we could use L1-regularization:

$$f(W,Z) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda_1}{2}\sum_{i=1}^{n}\|z_i\|_1 + \frac{\lambda_2}{2}\sum_{j=1}^{d}\|w_j\|_1$$

  – Called sparse coding (L1 on 'Z') or sparse dictionary learning (L1 on 'W').
- Disadvantage of using L1-regularization over non-negativity:
  – Sparsity controlled by λ_1 and λ_2 so you need to set these.
- Advantage of using L1-regularization:
  – Negative coefficients usually make sense.
  – Sparsity controlled by λ_1 and λ_2, so you can control amount of sparsity.

Sparse Matrix Factorization

- Instead of non-negativity, we could use L1-regularization:

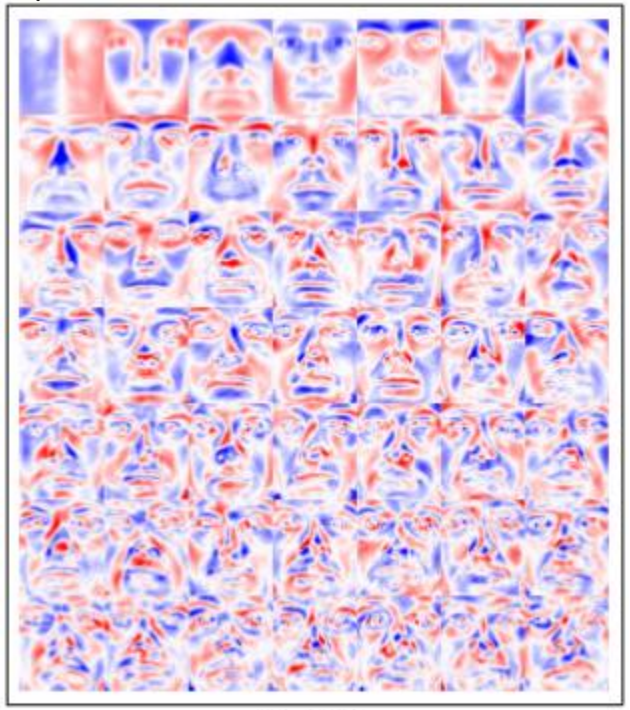
$$f(W,Z) = \frac{1}{2}\|ZW - X\|_F^2 + \frac{\lambda_1}{2}\sum_{i=1}^{n}\|z_i\|_1 + \frac{\lambda_2}{2}\sum_{j=1}^{d}\|w_j\|_1$$

  – Called sparse coding (L1 on 'Z') or sparse dictionary learning (L1 on 'W').
- Many variations exist:
  – Mixing L2-regularization and L1-regularization or making one a constraint.
  – K-SVD constrains each z_i to have at most 'k' non-zeroes:
    - K-means is special case where k = 1.
    - PCA is special case where k = d.

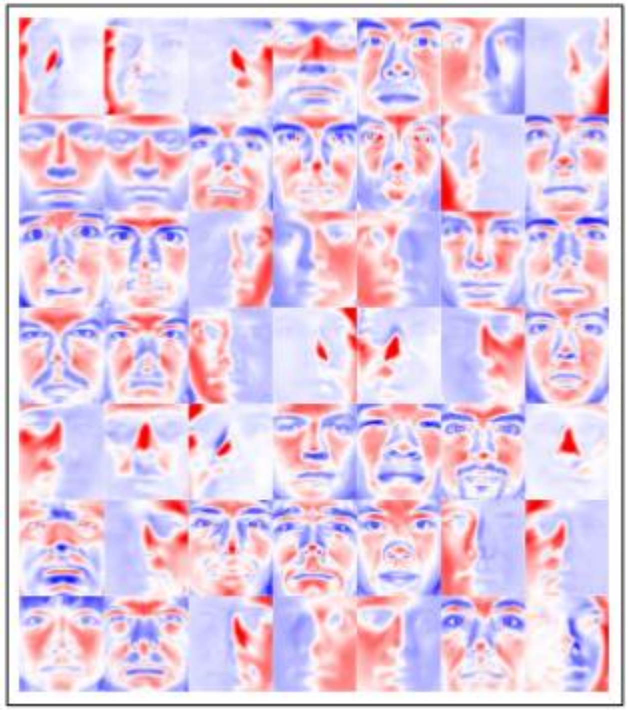
Matrix Factorization with L1-Regularization

blue: negative

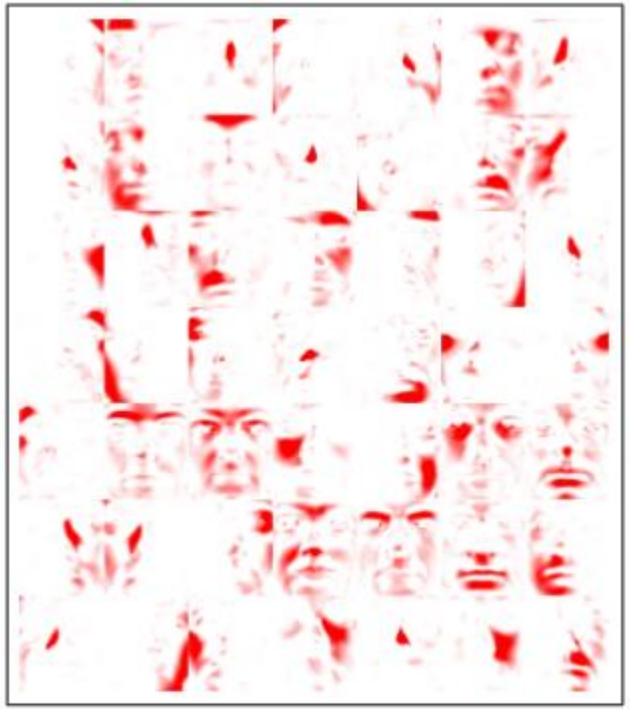
red: positive



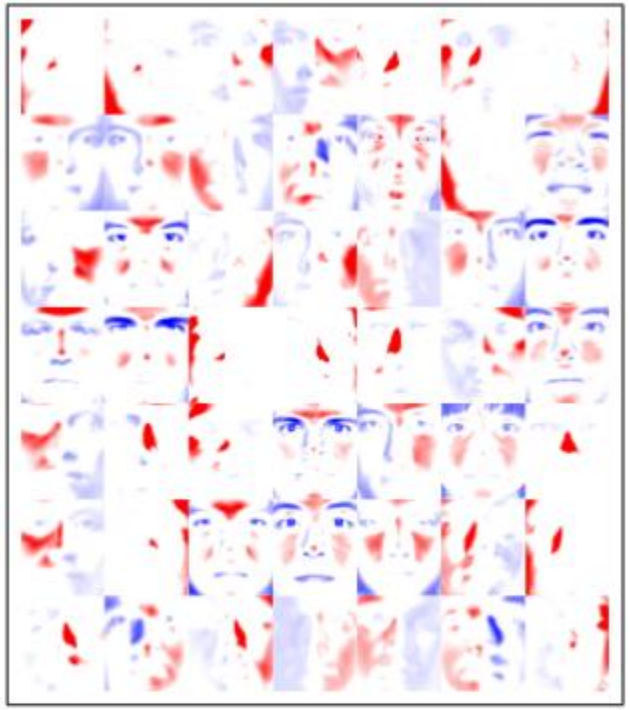
(a) PCA



(e) Dictionary Learning



(c) NMF



(d) SPCA, $\tau = 30\%$

PCA <u>without</u> orthogonality

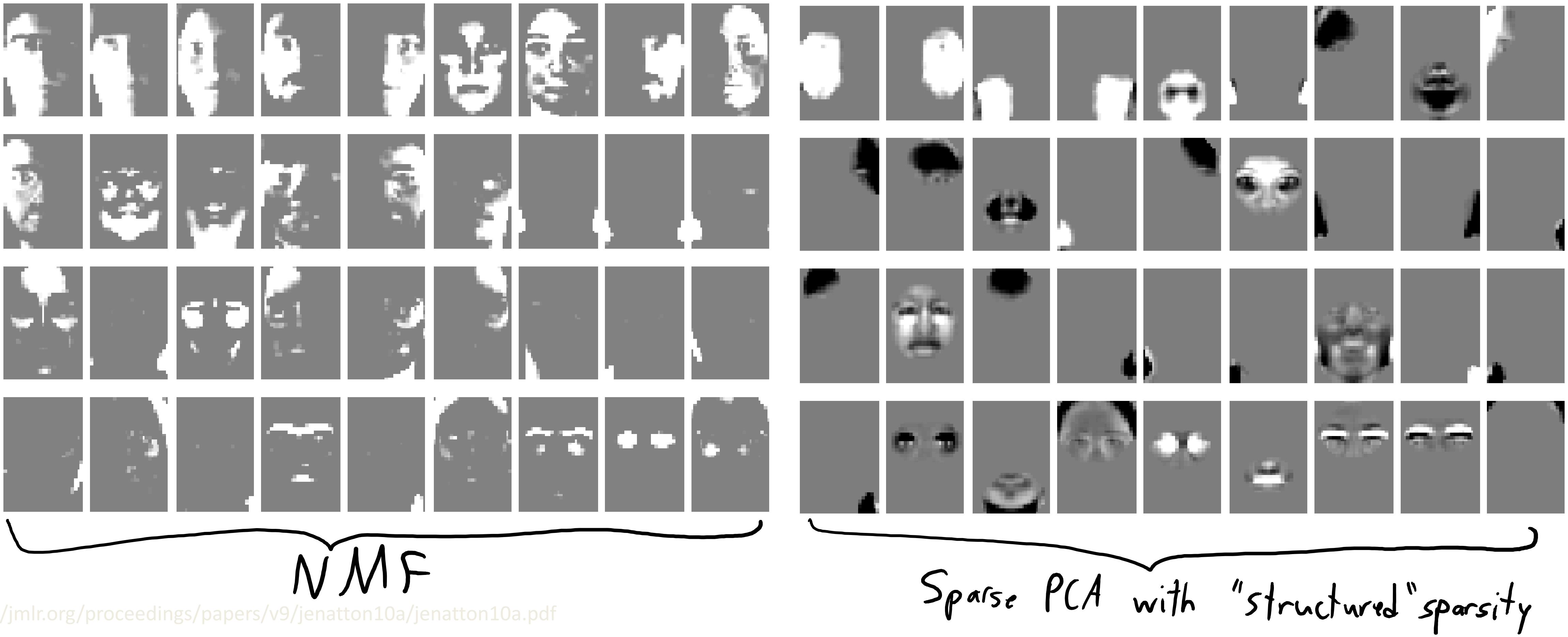
sparsity due to non-negativity

sparsity due to L_1-regularization

http://www.jmlr.org/papers/volume11/mairal10a/mairal10a.pdf

Recent Work: Structured Sparsity

- "Structured sparsity" considers dependencies in sparsity patterns.

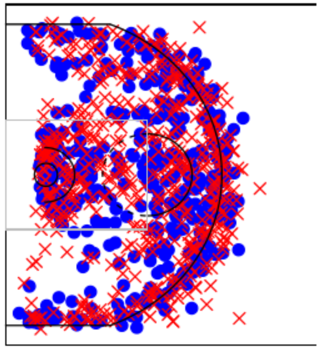


http://jmlr.org/proceedings/papers/v9/jenatton10a/jenatton10a.pdf

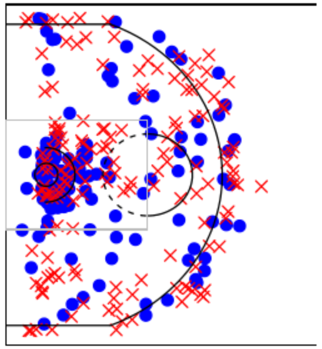
Application: Sports Analytics

- NBA shot charts:

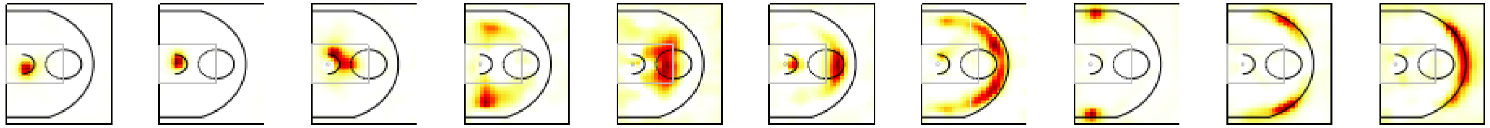
Stephen Curry (940 shots)



LeBron James (315 shots)



- NMF (using “KL divergence” loss with k=10 and smoothed data).
  - Negative values would not make sense here.



LeBron James	0.21	0.16	0.12	0.09	0.04	0.07	0.00	0.07	0.08	0.17
Brook Lopez	0.06	0.27	0.43	0.09	0.01	0.03	0.08	0.03	0.00	0.01
Tyson Chandler	0.26	0.65	0.03	0.00	0.01	0.02	0.01	0.01	0.02	0.01
Marc Gasol	0.19	0.02	0.17	0.01	0.33	0.25	0.00	0.01	0.00	0.03
Tony Parker	0.12	0.22	0.17	0.07	0.21	0.07	0.08	0.06	0.00	0.00
Kyrie Irving	0.13	0.10	0.09	0.13	0.16	0.02	0.13	0.00	0.10	0.14
Stephen Curry	0.08	0.03	0.07	0.01	0.10	0.08	0.22	0.05	0.10	0.24
James Harden	0.34	0.00	0.11	0.00	0.03	0.02	0.13	0.00	0.11	0.26
Steve Novak	0.00	0.01	0.00	0.02	0.00	0.00	0.01	0.27	0.35	0.34

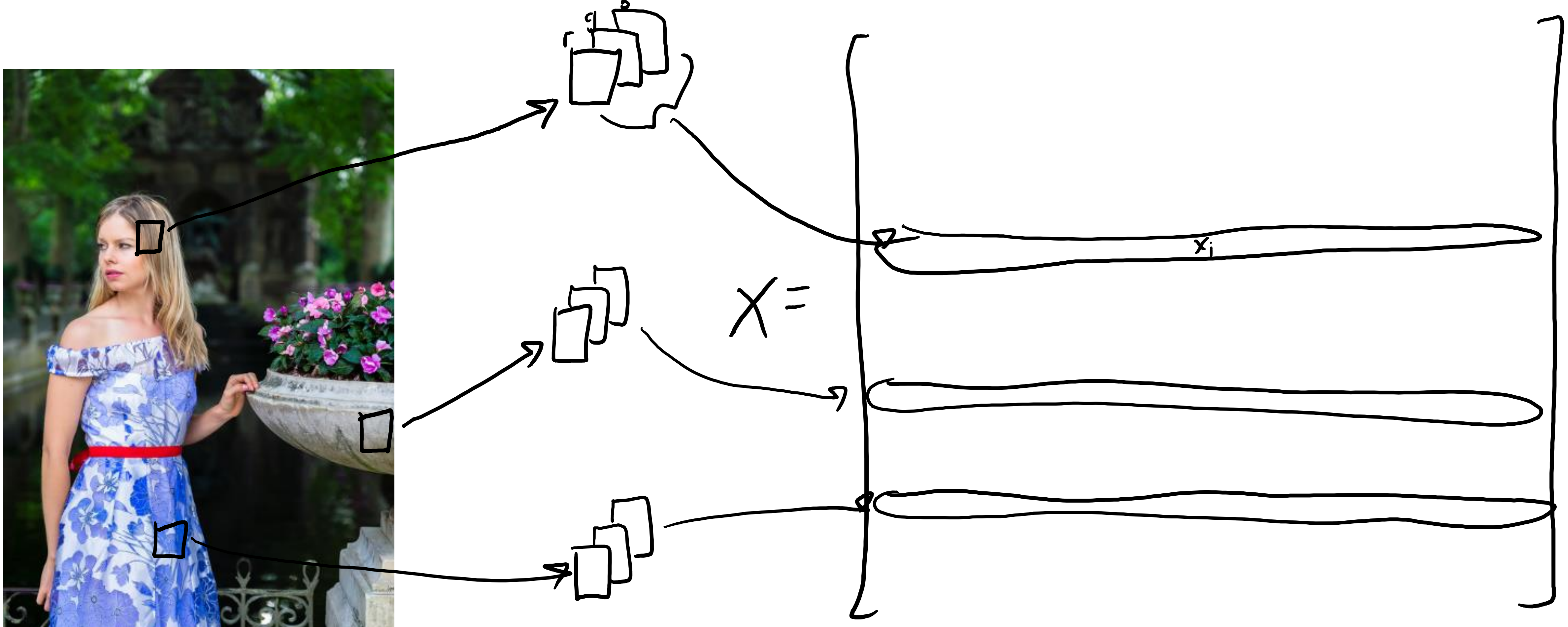
http://jmlr.org/proceedings/papers/v32/miller14.pdf

Application: Image Restoration

http://www.jmlr.org/papers/volume11/mairal10a/mairal10a.pdf

Latent-Factor Models for Image Patches

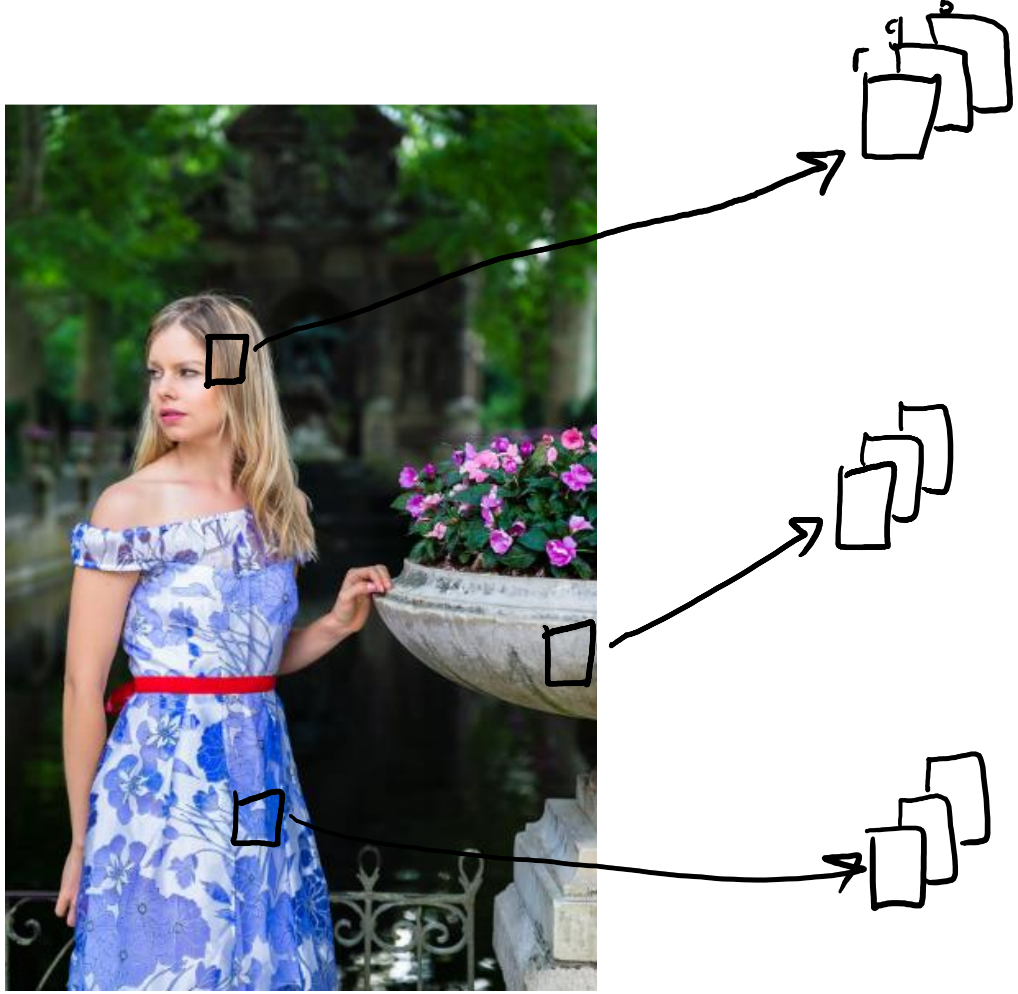
- Consider building latent-factors for general image patches:



Size of X: (image height) × (image width) by ((patch height) × (patch width) × 3)

Latent-Factor Models for Image Patches

- Consider building latent-factors for general image patches:

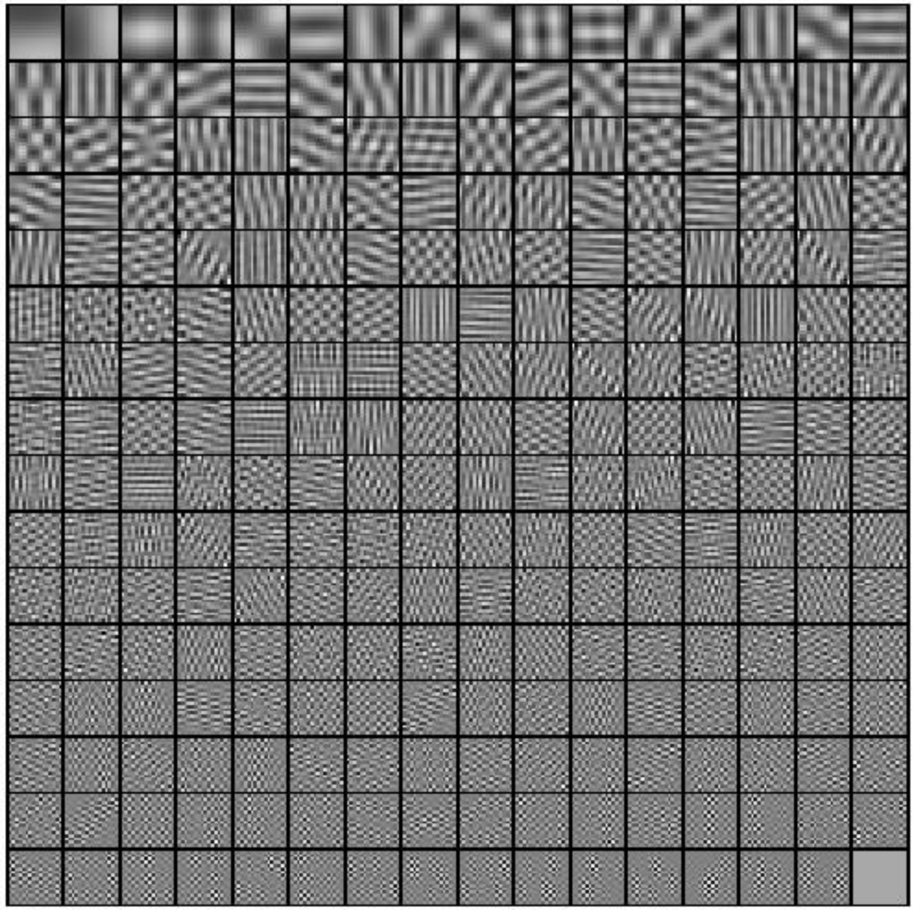


Typical pre-processing:

1. Usual variable centering
2. “Whiten” patches.

(remove correlations)

Latent-Factor Models for Image Patches

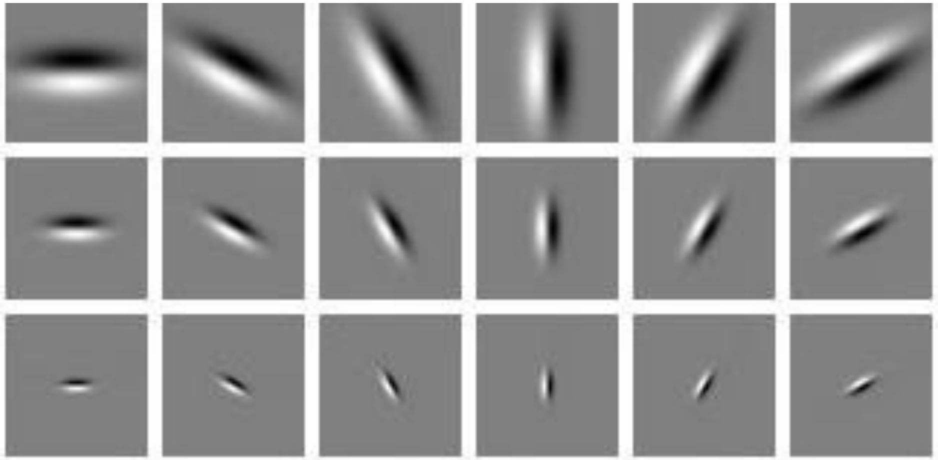


(b) Principal components.

Orthogonal bases don't seem right:

- Few PCs do almost everything.
- Most PCs do almost nothing.

We believe "simple cells" in visual cortex use:

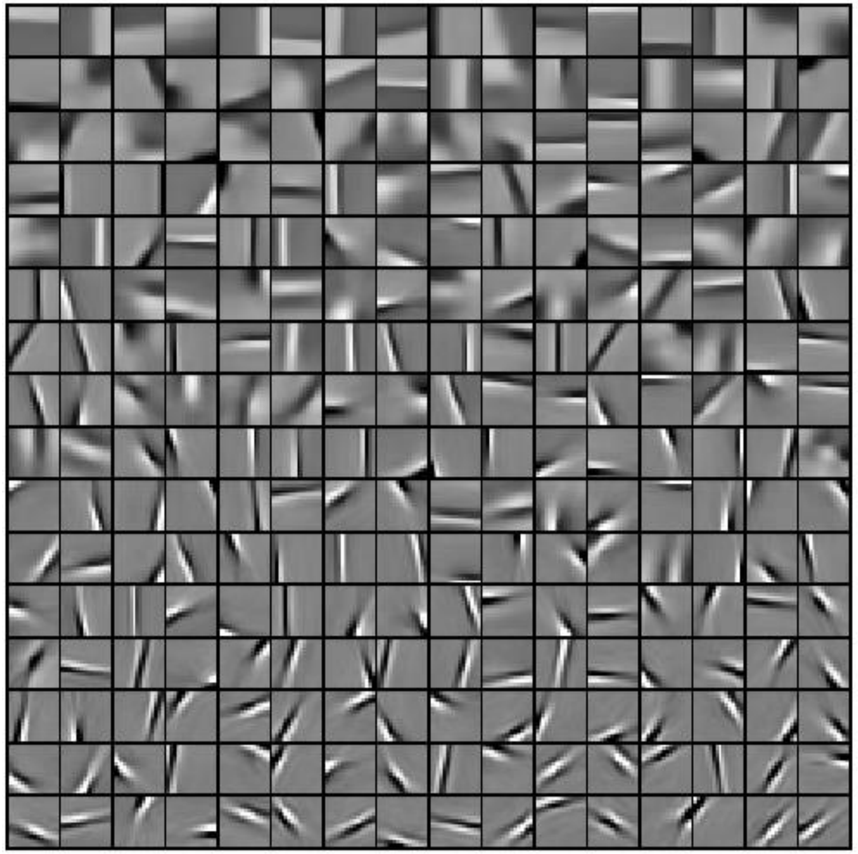


'Gabor' filters

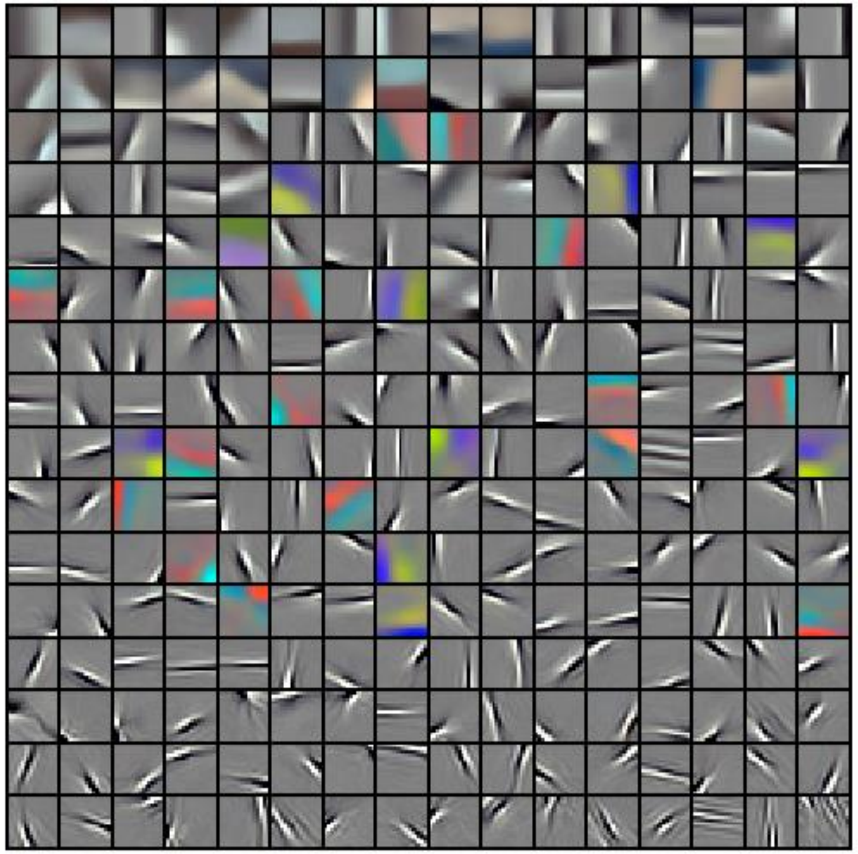
http://lear.inrialpes.fr/people/mairal/resources/pdf/review_sparse_arxiv.pdf
http://stackoverflow.com/questions/16059462/comparing-textures-with-opencv-and-gabor-filters

Latent-Factor Models for Image Patches

- Results from a sparse (non-orthogonal) latent factor model:



(a) With centering - gray.

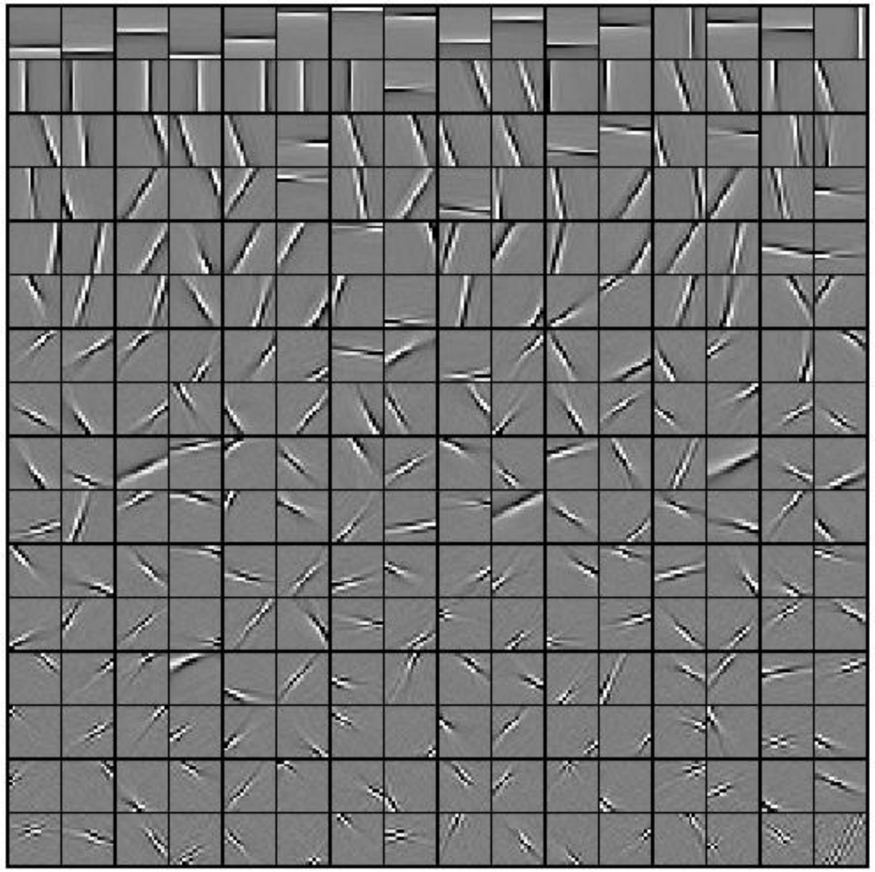


(b) With centering - RGB.

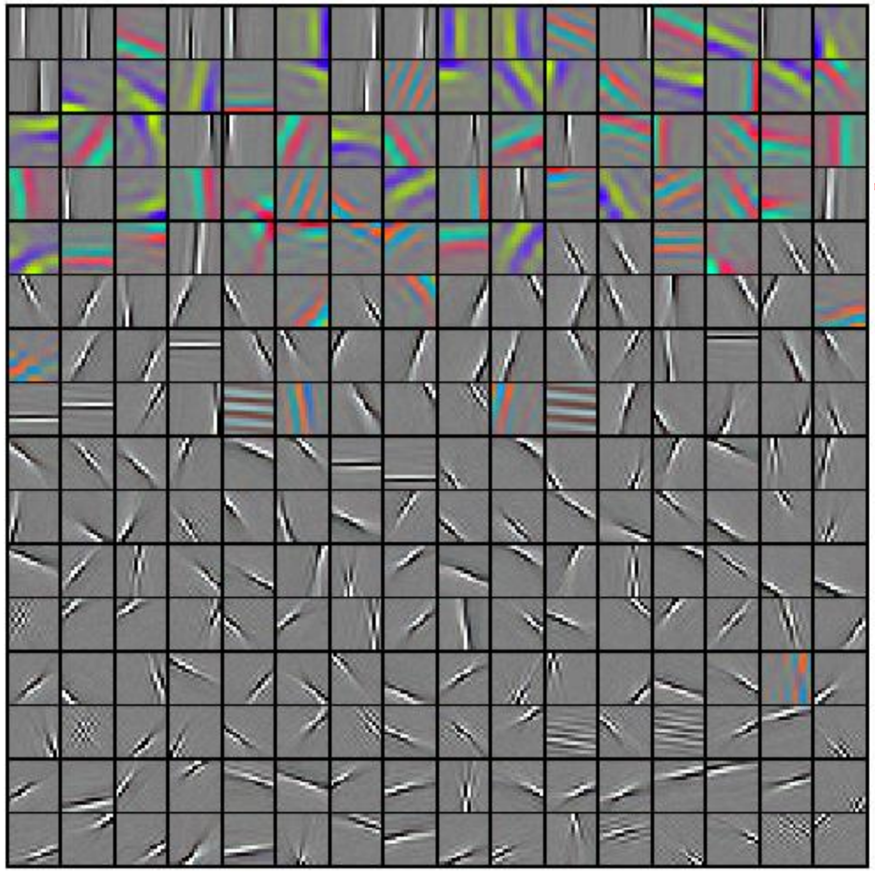
http://lear.inrialpes.fr/people/mairal/resources/pdf/review_sparse_arxiv.pdf

Latent-Factor Models for Image Patches

- Results from a "sparse" (non-orthogonal) latent-factor model:



(c) With whitening - gray.



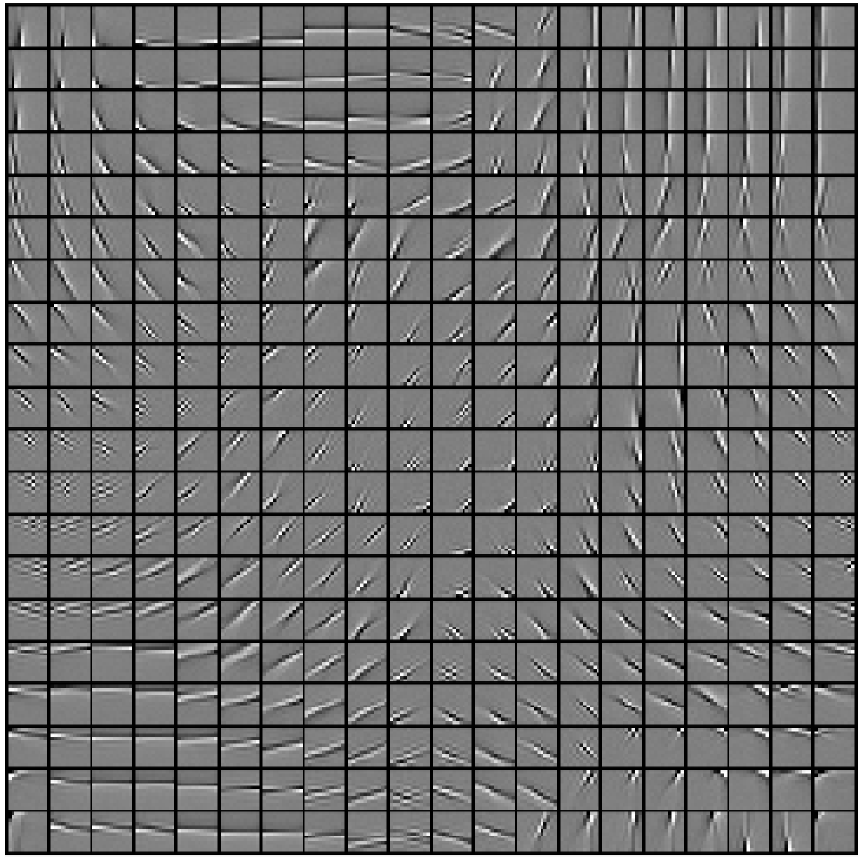
(d) With whitening - RGB.

"colour opponency"

http://lear.inrialpes.fr/people/mairal/resources/pdf/review_sparse_arxiv.pdf

Recent Work: Structured Sparsity

- Basis learned with a variant of "structured sparsity":



(b) With 4 × 4 neighborhood.

Similar to "cortical columns" theory in visual cortex.

http://lear.inrialpes.fr/people/mairal/resources/pdf/review_sparse_arxiv.pdf

Beyond Squared Error

- Our (unregularized) objective for latent-factor models (LFM):

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (w_j^T z_i - x_{ij})^2$$

- As before, there are squared error alternatives.
- We can get a LFM for binary x_{ij} using the logistic loss:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} \log(1+\exp(-x_{ij} w_j^T z_i))$$

Robust PCA

- Robust PCA methods use the absolute error:

$$f(W,Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} |w_j^T z_i - x_{ij}|$$

- Will be robust to outliers in the matrix 'X'.
- Encourages "residuals" r_{ij} to be exactly zero.
  - Non-zero r_{ij} are where the "outliers" are.

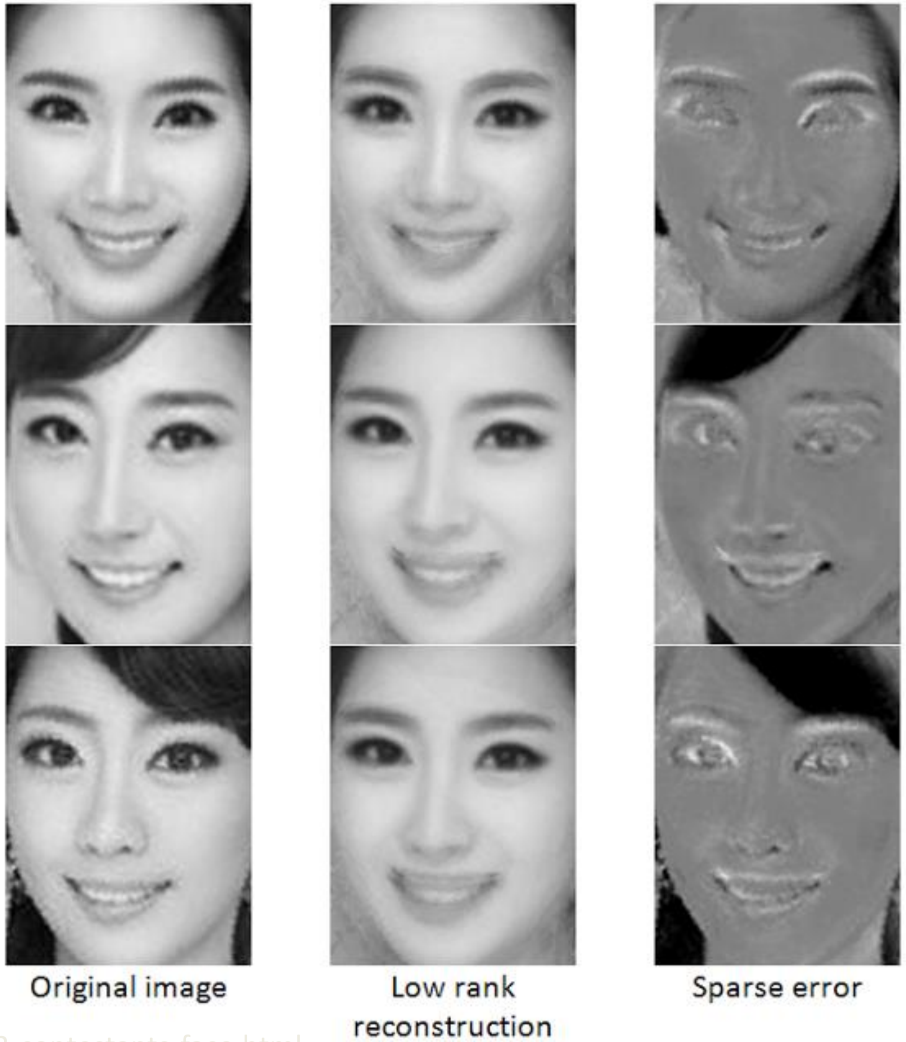
Applying robust PCA to video frames

x_{ij} $w_j^T z_i$ r_{ij}

http://statweb.stanford.edu/~candes/papers/RobustPCA.pdf

Robust PCA

- Miss Korea contestants and robust PCA:



http://jbhuang0604.blogspot.ca/2013/04/miss-korea-2013-contestants-face.html

Summary

- Non-negativity constraints lead to sparse solution.
- Projected gradient adds constraints to gradient descent.
- Non-orthogonal LFMs make sense in many applications.
- L1-regularization leads to other sparse LFMs.
- Robust PCA allows identifying certain types of outliers.

- Next time: predicting which movies you are going to like.