#### Machine learning for vision Winter 2015

Roland Memisevic

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# Gaussians and independence

Spherical Gaussians have independent marginals:

$$\rho(x_1, ..., x_n) = \frac{1}{(2\pi)^{\frac{n}{2}}} \exp\left(-\frac{1}{2} ||\mathbf{x}||^2\right) \\
= \prod_i \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2} x_i^2\right)$$

- ▶ So for Gaussian data, whitening will give us the independent components.
- ▶ For non-Gaussian data this is *not* the case.

# Correlation vs. dependence

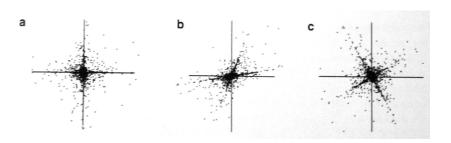
Statistical independence implies uncorrelatedness.

Uncorrelatedness does not imply statistical independence.

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# A counter example

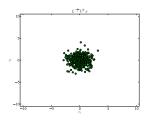


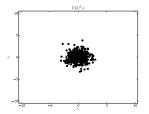
- a: Independent variables.
- b: A linear combination: not independent.
- c: After whitening the linear combination: still not independent.

from: Natural Image Statistics (Hyvarinen, Hurri, Hoyer; 2009)



# Uncorrelatedness is not independence





- ▶ Any orthogonal transformation of white data is white.
- ► Therefore, PCA and ZCA are just two out of infinitely many whitening matrices.
- How can we find the matrix that maximizes independence?
- ► Since independence implies uncorrelatedness, it must still be a whitening matrix.

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# Independent components analysis

- ► Here, A and W are square matrices. We will later extend this to over- or undercomplete representations.
- Multiplying any component  $s_i$  by some scalar will have no effect if we divide the corresponding  $A_i$  by the same number.
- So we may assume the rows of *A* to have some fixed length.
- ➤ Applying the model to already whitened components, **z**, (e.g. from PCA or ZCA), will greatly simplify learning because it allows us to search for **A** among orthogonal matrices.

#### Independent components analysis

► The ICA generative model: We have independent "source" variables  $s_i$ , which get mixed to yield the observed data

$$x = As$$

with

$$p(s_1,\ldots,s_n)=\prod_i p_i(s_i)$$

▶ The corresponding analysis equation is thus

$$\mathbf{s} = \mathbf{W}^{\mathrm{T}} \mathbf{x}$$

with 
$$\boldsymbol{W}^{\mathrm{T}} = \boldsymbol{A}^{-1}$$



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#### Maximum likelihood ICA

#### Densities under linear transformation

Given some random vector  $\mathbf{s}$  with density  $p_s(\mathbf{s})$ , the density of

$$x = Ms$$

is:

#### Maximum likelihood ICA

#### Densities under linear transformation

Given some random vector  $\mathbf{s}$  with density  $p_s(\mathbf{s})$ , the density of

$$x = Ms$$

is:

$$\rho_{x}(\boldsymbol{x}) = \frac{1}{|\det \boldsymbol{M}|} \rho_{s}(\boldsymbol{M}^{-1}\boldsymbol{x})$$

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#### Maximum likelihood ICA

▶ For IID observations, we get the following likelihood:

$$L(\boldsymbol{W}) = \prod_{t=1}^{T} p(\boldsymbol{x}_{t}) = \prod_{t=1}^{T} \left[ |\det \boldsymbol{W}| \prod_{i=1}^{n} p_{i}(\boldsymbol{w}_{i}^{\mathrm{T}} \boldsymbol{x}_{t}) \right]$$

► The log-likelihood is

$$\log L(\boldsymbol{W}) = T \log |\det \boldsymbol{W}| + \sum_{i=1}^{n} \sum_{t=1}^{T} \log p_{i}(\boldsymbol{w}_{i}^{T}\boldsymbol{x}_{t})$$

▶ For whitened data, **W** must be orthonormal, so

$$|\det oldsymbol{W}|=1$$

▶ In that case it is sufficient to maximize

$$\sum_{i=1}^{n} \sum_{t=1}^{T} \log p_i(\boldsymbol{w}_i^{\mathrm{T}} \boldsymbol{z}_t)$$

#### Maximum likelihood ICA

- ▶ For the ICA model, plug in  $\mathbf{A} = \mathbf{W}^{-T}$  for  $\mathbf{M}$ .
- We have

$$\frac{1}{\det \boldsymbol{A}} = \frac{1}{\det \boldsymbol{W}^{-T}} = \frac{1}{\det \boldsymbol{W}^{-1}} = \det \boldsymbol{W}$$

► So we can write

$$p(\mathbf{x}) = \big|\det \mathbf{W} \big| p(\mathbf{W}\mathbf{x}) = \big|\det \mathbf{W} \big| \prod_{i=1}^n p_i ig(\mathbf{w}_i^{\mathrm{T}}\mathbf{x}ig)$$



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#### Maximum likelihood ICA

This leads to the constrained optimization problem

minimize 
$$\sum_{t} \sum_{i} \phi(\boldsymbol{w}_{i}^{\mathrm{T}} \boldsymbol{z}_{t})$$
s.t. 
$$\boldsymbol{W}^{\mathrm{T}} \boldsymbol{W} = \boldsymbol{I}$$

where  $-\phi(s_i) = \log p(s_i)$  is the log-pdf of the independent sources.

▶ How to choose  $\phi(s_i)$  ?

#### Maximum likelihood for Gaussian sources



- ▶ The independent Gaussian is spherically symmetric.
- So rotation (orthogonal *W*) will have no effect on the objective.
- Any non-Gaussian source distribution will.

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#### Gaussian scale mixtures

- ► A possible explanation for super-Gaussianity in natural images is that any one feature may occur at different (brightness-)scales.
- ▶ We can model an image patch using a Gaussian g<sub>i</sub> whose value is modulated by some independent scale-variable d<sub>i</sub>:

$$s_i = g_i d_i$$

- ► This yields a super-Gaussian distribution, because  $p(s_i)$  will be a superposition of Gaussians each with different variance.
- ► In fact, contrast normalization seems to reduce sparsity (a bit).

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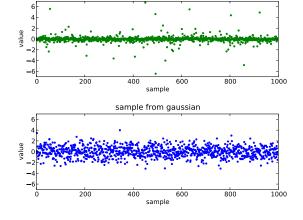
- ▶ Three possible forms of non-Gaussianity are
  - 1. Super-Gaussian (= *sparsity*): Distribution is peaked at zero (positive kurtosis)
  - 2. Sub-Gaussian: Distribution is "flat" at zero (negative kurtosis)
  - 3. Skew: Distribution is unsymmetric.
- ► Of these, super-Gaussianity is generally assumed to be the best match for (most) image data.
- Sparse representations are beneficial in many ways, so it is a natural choice of non-Gaussian density also for practical reasons.



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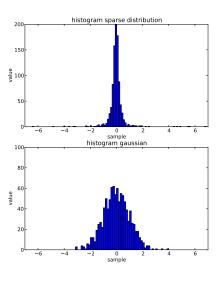
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# Sparseness



- ► Top: Samples from a student-T-distribution (sparse)
- ► Bottom: Samples from a normal distribution of the same variance (not sparse).

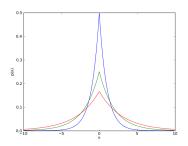
# Histograms



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# Sparse source densities



► A popular choice of sparse source density is the zero-mean Laplacian:

$$p(s_i) = \frac{1}{2h} \exp\left(-\frac{|s_i|}{h}\right)$$

► Another, differentiable, one is the log cosh function.

# Sparse does not mean "small values"

- Sparsity should not be confused with "small".
- ► A normal distribution may be scaled to take on small values, too. This doesn't make it sparse.
- Sparsity should always be thought of as relative to a given variance.



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# Sparse coding

 With a Laplacian source density, the optimization problem becomes

minimize 
$$\sum_{t} \sum_{i} |\boldsymbol{w}_{i}^{\mathrm{T}} \boldsymbol{z}_{t}|$$
s.t. 
$$\boldsymbol{W}^{\mathrm{T}} \boldsymbol{W} = \boldsymbol{I}$$

► This can be solved by alternating gradient steps with projections to enforce the constraint.

# Orthogonality from reconstruction error

► An alternative to solving the constrained optimization problem is to enforce the orthogonality constraint

$$\mathbf{W}^{-1} = \mathbf{W}^{\mathrm{T}}$$

implicitly.

By adding a reconstruction term we can encourage this as follows:

$$\text{minimize} \qquad \sum_t \| \boldsymbol{W} \boldsymbol{W}^{\mathrm{T}} \boldsymbol{z}_t - \boldsymbol{z}_t \|^2 + \lambda \sum_t \sum_i |\boldsymbol{w}_i^{\mathrm{T}} \boldsymbol{z}_t|$$

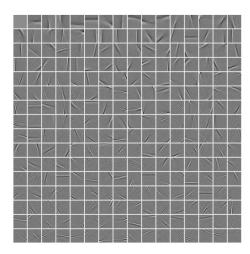
Note that we have  $\mathbf{A} = \mathbf{W}$  now.

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#### **ICA** filters



from: Natural Image Statistics (Hyvarinen, Hurri, Hoyer; 2009)

#### Search based inference

- ► All of the above versions of ICA make use of an encoder (*W*) and decoder (*A*).
- ► An alternative formulation one can find in the literature is to ignore the decoder and to *search* for the right **s** during learning (and inference as well):

minimize 
$$\sum_{t} \| \boldsymbol{A}^{\mathrm{T}} \boldsymbol{s}_{t} - \boldsymbol{z}_{t} \|^{2} + \sum_{t} \sum_{i} |\boldsymbol{s}_{ti}|$$

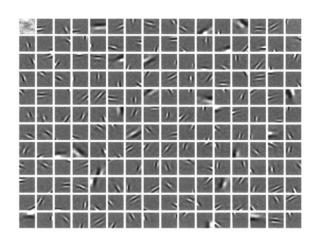
where the optimization is over  $\boldsymbol{A}$  and all the  $\boldsymbol{s_t}$  during training and over  $\boldsymbol{s}$  during inference.

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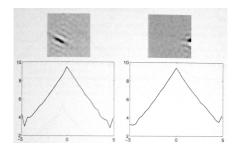
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# Sparse coding components (Olshausen/Field)

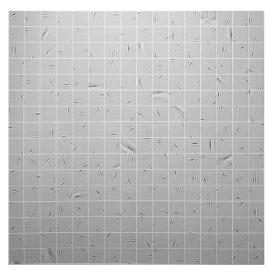


# Estimating the source densities



- One can estimate the source densities from data as well.
- It turns out that not all components are sparse.
- ▶ The DC component, for example, tends to be sub-Gaussian.
- So to keep it or not can make a difference in practice!

# Example analysis filters



from: Natural Image Statistics (Hyvarinen, Hurri, Hoyer; 2009)

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# Relation between analysis and synthesis weights

 $\triangleright$  Since the  $s_i$  are independent and have unit variance, the covariance matrix, **C**, over input images can be written

$${m C} = {m A}{m A}^{
m T}$$

From this, and  $\mathbf{W} = \mathbf{A}^{-1}$ , it follows that:

$$\mathbf{A}^{\mathrm{T}} = \mathbf{I} \mathbf{A}^{\mathrm{T}}$$

$$= (\mathbf{A}^{-1} \mathbf{A}) \mathbf{A}^{\mathrm{T}}$$

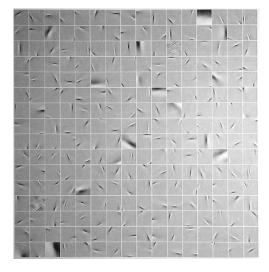
$$= \mathbf{W}^{\mathrm{T}} \mathbf{A} \mathbf{A}^{\mathrm{T}}$$

$$= \mathbf{W}^{\mathrm{T}} \mathbf{C}$$

▶ In other words, synthesis weights,  $\mathbf{A} = \mathbf{C}\mathbf{W}$ , are equal to input covariance times analysis weights!

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# Example synthesis filters



from: Natural Image Statistics (Hyvarinen, Hurri, Hoyer; 2009)

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# Frequency channels

- The emergence of bandpath filters from whitening shows that 2d Fourier features (frequencies/orientations) are uncorrelated components.
- The emergence of Gabor features from ICA shows that (frequencies/orientations/positions) are independent components.
- What independence/sparsity adds is *locality*.
- ► This suggests that natural images are mainly invariant to *local translations*.



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#### Information theoretic interpretation

➤ To measure the independence of the sources we can use *mutual information* as follows:

$$\begin{aligned}
& \operatorname{MI}(\boldsymbol{s}_{1}, \dots, \boldsymbol{s}_{K}) \\
&= \int_{\boldsymbol{s}_{1}, \dots, \boldsymbol{s}_{K}} p(\boldsymbol{s}_{1}, \dots, \boldsymbol{s}_{K}) \log \frac{p(\boldsymbol{s}_{1}, \dots, \boldsymbol{s}_{K})}{p(\boldsymbol{s}_{1}) \cdots p(\boldsymbol{s}_{K})} d\boldsymbol{s}_{1} \cdots d\boldsymbol{s}_{K} \\
&= \sum_{i=1}^{K} H(\boldsymbol{s}_{i}) - H(\boldsymbol{s}) \\
&= \sum_{i=1}^{K} H(\boldsymbol{w}_{i}^{T}\boldsymbol{z}) - H(\boldsymbol{W}\boldsymbol{z}) \end{aligned}$$

- ► For orthogonal *W*, the joint entropy is constant.
- So to minimize MI, minimize the entropies of the individual components. → Make them less Gaussian!

#### Information theoretic interpretation

► To measure the independence of the sources we can use *mutual information* as follows:

$$MI(s_1, ..., s_K)$$

$$= \int_{s_1, ..., s_K} p(s_1, ..., s_K) \log \frac{p(s_1, ..., s_K)}{p(s_1) \cdots p(s_K)} ds_1 \cdots ds_K$$

$$= \sum_{i=1}^K H(s_i) - H(s)$$

$$= \sum_{i=1}^K H(\mathbf{w}_i^T \mathbf{z}) - H(\mathbf{W} \mathbf{z})$$

- For orthogonal **W**, the joint entropy is constant.
- ► So to minimize MI, minimize the entropies of the individual components.

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#### Infomax ICA

- Yet another information theoretic approach to ICA can be derived as follows:
- Maximum likelihood ( $\hat{=}$  minimum entropy) under some density f(x) can also be viewed as maximizing the *derivative of its cumulative distribution*  $F(x) = \int f(x) dx$
- But this is equivalent to making the values under the cumulative distribution more uniform. (Also known as "maximum spacing" estimation in the literature.)
- ▶ To maximize uniformity of F(x) we may *maximize* the entropy of the random variable F(x) ( $\widehat{=}$  minimize its likelihood).
- (We can make the same argument for multivariate data x)

#### Infomax ICA

- ▶ But F(x) is a deterministic function of x, so we can write its density as a function of x.
- ► In particular, the transformation of densities under non-linear transformations is

$$p_F(F(\boldsymbol{x})) = \frac{1}{|\det J(\boldsymbol{x})|} p_{\boldsymbol{x}}(\boldsymbol{x})$$

where  $J(\mathbf{x}_t)$  is the Jacobian of  $F(\mathbf{x})$  at  $\mathbf{x}$ 

▶ By eliminating terms that do not depend on the parameters of *F*, we get the optimization problem:

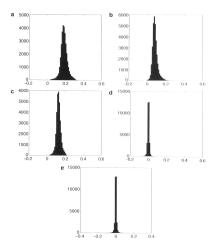
$$\text{minimize } -\sum_t \log |\det J(\boldsymbol{x}_t)|$$

► (Bell, Sejnowski 1997)

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#### Non-linear correlations, limitations of ICA



- a: f(s) = |s|
- ▶ b:  $f(s) = s^2$
- c: f(s) = |s| > 1
- ▶ d: f(s) = sign(s)

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• e:  $f(s) = s^3$ 

from: Natural Image Statistics (Hyvarinen, Hurri, Hoyer; 2009)

#### Non-linear correlations, limitations of ICA

For independent random variables,  $s_1$ ,  $s_2$ , the following must be true:

$$\operatorname{cov}(f(s_1),f(s_2))=0$$

where *f* is any non-linear function.

- ► There are infinitely many *f*-functions we could choose from.
- ► This hints at the fact that a linear ICA transformation with its  $n^2$  parameters may not be able to yield perfectly independent components.



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# Blind source separation

- ► A classic application of ICA is separating (unmixing) audio sources:
- ► Eg. http://cnl.salk.edu/~ tewon/Blind/blind audio.html