

Why Hebbian learning can implement PCA

• Write w(t) in terms of the eigenvectors of *C*:

$$\boldsymbol{w}(t) = \sum_{k} a_{k}(t) \boldsymbol{v}_{k} = \boldsymbol{e}^{\eta C t} \boldsymbol{w}(0)$$
$$= \boldsymbol{e}^{\eta C t} \sum_{k} a_{k}(0) \boldsymbol{v}_{k}$$
$$= \sum_{k} a_{k}(0) \boldsymbol{e}^{\eta C t} \boldsymbol{v}_{k}$$
$$= \sum_{k} a_{k}(0) \boldsymbol{e}^{\eta \lambda_{k} t} \boldsymbol{v}_{k}$$

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Why Hebbian learning can implement PCA

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- "But ||w|| will grow."
 Solution: Renormalize after every step (Oja's rule).
- "What about the other eigenvectors v₂,..., v_D?" Solution: Orthogonalize after each step (Sanger's rule).
- With some small modifications (for example, non-linear output nonlinearity) Hebbian learning can implement sparse coding, too.

Why Hebbian learning can implement PCA

- Assume $\lambda_1 > \ldots > \lambda_D$
- Then we have

$$w(t) = \sum_{k} a_{k}(t) e^{\eta \lambda_{k} t} \mathbf{v}_{k}$$
$$= e^{\eta \lambda_{1} t} [a_{1}(0) \mathbf{v}_{1} + \sum_{k=2}^{D} a_{k}(0) e^{-\eta t(\lambda_{1} - \lambda_{k}) \mathbf{v}_{k}}]$$
$$\approx a_{1}(0) e^{\eta \lambda_{1} t} \mathbf{v}_{1}$$

 $\lim_{t\to\infty}\frac{\boldsymbol{w}(t)}{\|\boldsymbol{w}(t)\|}=\pm\boldsymbol{v}_1$

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Probabilistic PCA

 One can define PCA also as a probabilistic latent variable model (Tipping, Bishop; 1999).

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Assume a Gaussian prior distribution over latent variables

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0},\mathbf{I})$$

and a Gaussian conditional distribution over images \boldsymbol{x}

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^{2}\mathbf{I})$$

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Probabilistic PCA $\frac{1}{p(x)} + \frac{1}{p(x)} + \frac{1}{p(x)$

draw from a low-dimensional Gaussian in the latent space, and then draw the observation from a *D*-dimensional conditional Gaussian whose mean depends on the latent variable.

Gaussians and independence

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Spherical Gaussians have independent marginals:

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

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- Implications:
 - 1. For Gaussian distributed data, whitening amounts to extracting the independent components.
 - 2. For Gaussian distributed data, uncorrelatedness implies independence.
- ► For non-Gaussian distributions these are *not* true.

Probabilistic PCA

• The backward mapping follows from Bayes' rule:

$$p(\mathbf{z}|\mathbf{x}) = rac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{\int_{\mathbf{z}} p(\mathbf{x}|\mathbf{z})p(\mathbf{z})\mathrm{d}\mathbf{z}}$$

Plugging in the Gaussian distributions yields

$$p(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}|\mathbf{M}^{-1}\mathbf{W}^{\mathrm{T}}(\mathbf{x}-\boldsymbol{\mu}), \sigma^{-2}\mathbf{M})$$

with $\mathbf{M} = \mathbf{W}^{\mathrm{T}}\mathbf{W} + \sigma^{2}\mathbf{I}$

The marginals turn out to be Gaussian, too:

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) \, \mathrm{d}\mathbf{z} = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{W}\mathbf{W}^{\mathrm{T}} + \sigma^{2}\mathbf{I})$$

 This is simply a Gaussian, whose covariance matrix is the outer product of two low-rank matrices (plus noise).

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A counter example



- a: Independent variables.
- b: A linear combination: not independent.
- c: Linear combination after whitening: not independent.

Uncorrelatedness is not independence



- Recall that any orthogonal transformation of white data is white.
- PCA and ZCA are two of the infinitely many example whitening matrices.
- How can we find the one that maximizes independence?

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Independent components analysis

 Generative model: We have independent "source" variables s_i, which get mixed to yield the observed data:

 $\pmb{x}=\pmb{A}^{\mathrm{T}}\pmb{s}$

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

The analysis equation is:

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

For images it can be convenient to write this as

$$I(x, y) = \sum_{i=1}^{n} A_i(x, y) s_i$$
$$s_i = \sum_{x, y} W_i(x, y) I(x, y)$$

► Learning: Find A and W as well as all the **s**.

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Finding independent components is whitening



- Independence does imply uncorrelatedness.
- So the linear transformation that makes data independent (if it exists) must still be a whitening matrix!

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Independent components analysis

- Instead of the original images, *I*, we typically use the whitened components, *z*, (from PCA or ZCA) as the input data.
- Multiplying any component s_i by some scalar will have no effect if we divide the corresponding A_i by the same number.
- One way to fix this is by constraining *A*.
- In general, we also have to assume that $A = W^{-1}$.
- A and W need to be square matrices. We will relax that assumption in the future.

Implication for feature learning

- Most popular feature learning models (auto-encoder networks, k-means, restricted Boltzmann machines, etc.) utilize "tied weights".
- This means that the encoder weights are the transpose of the decoder weights:

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

- But this means that $W^{T}W = I$, so W is orthogonal.
- So these models are likely to work well only on whitened data!?

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Maximum likelihood ICA

The log-likelihood is

$$\log L(\boldsymbol{w}_1,\ldots,\boldsymbol{w}_n) = T \log \big| \det W \big| + \sum_{i=1}^n \sum_{t=1}^T \log p_i(\boldsymbol{w}_i^T \boldsymbol{x}_t)$$

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 If we apply this to pre-whitened data z, then W must be orthonormal, so

$$|\det W| = 1$$

In this case we may maximize:

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

Maximum likelihood ICA

 Since we assume independence of the s_i, we can write the pdf of the observations as

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

► For IID observations, we get the following likelihood:

$$L(\boldsymbol{w}_1,\ldots,\boldsymbol{w}_n) = \prod_{t=1}^T p(\boldsymbol{x}_t) = \prod_{t=1}^T \left[\left| \det W \right| \prod_{i=1}^n p_i(\boldsymbol{w}_i^T \boldsymbol{x}_t) \right]$$

Densities under linear transformation

Under a linear transformation $\boldsymbol{y} = \boldsymbol{W}\boldsymbol{x}$, the density $p_x(\boldsymbol{x})$ turns into

 $|\det W| \rho_x(W\mathbf{x})$

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Maximum likelihood ICA

 We can rewrite the constrained optimization problem as

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 $\phi() = -\log p_i()$ is some negative, non-Gaussian log-pdf.

 We just need to choose appropriate source densities...

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Gaussian scale mixtures

- One 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_i whose value is modulated by some independent scale-variable d_i:

$$s_i = g_i d_i$$

- 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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Sparse coding

 With this source density, the optimization problem turns into

 This can be solved by alternating gradient steps and projections that enforce the constraint.

Reconstruction error

 An alternative to solving a constrained optimization problem is to enforce the constraint

$$\boldsymbol{W}^{\mathrm{T}}\boldsymbol{W} = \boldsymbol{I} \Leftrightarrow \boldsymbol{W}^{-1} = \boldsymbol{W}^{\mathrm{T}}$$

implicitly.

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

Minimize
$$\sum_{t} \|\boldsymbol{W}\boldsymbol{W}^{\mathrm{T}}\boldsymbol{z}_{t} - \boldsymbol{z}_{t}\|^{2} + \sum_{t} \sum_{i} |\boldsymbol{w}_{i}^{\mathrm{T}}\boldsymbol{z}_{t}|$$

We may even separate encoder and decoder weights:

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Minimize

ze
$$\sum_{t} \|\boldsymbol{A}\boldsymbol{W}^{\mathrm{T}}\boldsymbol{z}_{t} - \boldsymbol{z}_{t}\|^{2} + \sum_{t} \sum_{i} |\boldsymbol{w}_{i}^{\mathrm{T}}\boldsymbol{z}_{t}|$$

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ICA filters



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Reconstruction error

In the literature one frequently finds

Minimize $\sum_{t} \|\boldsymbol{A}\boldsymbol{s}_{t} - \boldsymbol{z}_{t}\|^{2} + \sum_{t} \sum_{i} |\boldsymbol{s}_{i}|$

where the optimization is over both A and s.

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Sparse coding components (Olshausen/Field)



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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.

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So to keep it or not can make a difference in practice!

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Example analysis filters



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Relation between analysis and synthesis weights

• If the s_i are independent and have unit variance, it holds (exercise):

$$\operatorname{cov}((x,y),(x',y')) = \sum_{i} A_{i}(x,y)A_{i}(x',y')$$

Therefore:

$$\sum_{x',y'} \operatorname{cov}((x, y), (x', y')) W_i(x', y')$$

= $\sum_{x',y'} \sum_j A_j(x, y) A_j(x', y') W_i(x', y')$
= $\sum_i A_j(x, y) \sum_{x',y'} A_j(x', y') W_i(x', y') = A_i(x, y)$

 Multiplying by the covariance matrix is lowpass-filtering: (ロト・日本・日本・日本・1日本)

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Example synthesis filters



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Information theoretic interpretation

One can use the *mutual information* to measure independence of the s_i:

$$I(s_1, \dots, s_n) = \int_{s_1, \dots, s_n} p(s_1, \dots, s_n) \log \frac{p(s_1, \dots, s_n)}{p(s_1) \cdots p(s_n)}$$
$$= \sum_{i=1}^n H(s_i) - H(s)$$
$$= \sum_{i=1}^n H(w_i^{\mathrm{T}} z) - H(W z)$$

- ► For orthogonal *W*, the last term is constant.
- To minimize MI, minimize the entropy of individual components!
- To minimize their entropy, make them less Gaussian!

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