

A Direct Approach to ICA(I)

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A Direct Approach to ICA

- ▶ R package: ProDenICA

By definition, independent components have a joint product density:

$$f_S(s) = \prod_{j=1}^p f_j(s_j)$$

In the next slides, we present an approach that estimates this density directly using generalized additive models.

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In the spirit of representing departures from Gaussianity, we represent each f_j as

$$f_j(s_j) = \phi(s_j)e^{g_j(s_j)}$$

a tilted Gaussian density.

- ▶ ϕ : standard Gaussian density
- ▶ g_j satisfies the normalization conditions required of a density

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Assuming \mathbf{X} is pre-whitened, the log-likelihood for the observed data $\mathbf{X} = \mathbf{A}\mathbf{S}$ is:

$$\ell(\mathbf{A}, \{g_j\}_1^p; \mathbf{X}) = \sum_{i=1}^N \sum_{j=1}^p [\log \phi_j(a_j^T \mathbf{x}_i) + g_j(a_j^T \mathbf{x}_i)]$$

We wish to maximize the likelihood to the constraints that:

- ▶ \mathbf{A} is orthogonal
- ▶ g_j results in densities $f_j(s_j) = \phi(s_j)e^{g_j(s_j)}$.

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Without imposing any further restrictions on g_j , the model is over-parametrized. Therefore, we would instead maximize a regularized version:

$$\ell(\mathbf{A}, \{g_j\}_1^p; \mathbf{X}) = \sum_{i=1}^N \sum_{j=1}^p [\log \phi_j(a_j^T x_i) + g_j(a_j^T x_i)]$$

$$\sum_{j=1}^p \left[\frac{1}{N} \sum_{i=1}^N [\log \phi(a_j^T x_i) + g_j(a_j^T x_i)] - \int \phi(t) e^{g_j(t)} dt - \lambda_j \int \{g_j'''(t)\}^2(t) dt \right]$$

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$$\sum_{j=1}^p \left[\frac{1}{N} \sum_{i=1}^N [\log \phi(a_j^T x_i) + g_j(a_j^T x_i)] - \int \phi(t) e^{g_j(t)} dt - \lambda_j \int \{g_j'''(t)\}^2(t) dt \right]$$

- ▶ $\int \phi(t) e^{g_j(t)} dt$: enforces the density constraint $\int \phi(t) e^{g_j(t)} dt = 1$ on any solution \hat{g}_j
- ▶ $\lambda_j \int \{g_j'''(t)\}^2(t) dt$: a roughness penalty, which guarantees that the solution \hat{g}_j is a quartic-spline with knots at the observed values of $s_{ij} = a_j^T x_i$

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$$\sum_{j=1}^p \left[\frac{1}{N} \sum_{i=1}^N [\log \phi(a_j^T x_i) + g_j(a_j^T x_i)] - \int \phi(t) e^{g_j(t)} dt - \lambda_j \int \{g_j'''(t)\}^2(t) dt \right]$$

- It can be shown that the solution densities $\hat{f}_j = \phi e^{\hat{g}_j}$ each have mean zero and variance one.

As we increases λ_j , the solutions approach the standard Gaussian ϕ

Steps for the Product Density ICA Algorithm

► ProDenICA

$$\sum_{j=1}^p \left[\frac{1}{N} \sum_{i=1}^N [\log \phi(a_j^T x_i) + g_j(a_j^T x_i)] - \int \phi(t) e^{g_j(t)} dt - \lambda_j \int \{g_j'''(t)\}^2(t) dt \right]$$

We fit the functions g_j and directions a_j by optimizing the objective function in an alternating fashion, as described in the following:

1. Initialize \mathbf{A} (random Gaussian matrix followed by orthogonalization).
2. Alternate until convergence of \mathbf{A} :
 - (a) Given \mathbf{A} , optimize the objective function w.r.t. g_j (separately for each j)
 - (b) Given g_j , $j = 1, \dots, p$, perform one step of a fixed point algorithm towards finding the optimal A

Steps for the Product Density ICA Algorithm

- ▶ Step 2(a) amounts to a semi-parametric density estimation, which can be solved using a novel application of generalized additive models.
- ▶ For convenience, we extract one of the p separate problems:

$$\frac{1}{N} \sum_{i=1}^N [\log \phi(s_i) + g(s_i)] - \int \phi(t) e^{g(t)} dt - \lambda \int \{g'''(t)\}^2(t) dt$$

Steps for the Product Density ICA Algorithm

- For approximation, we construct a fine grid of L values s_ℓ^* in increments Δ covering the observed values s_i , and count the number of s_i in the resulting bins:

$$y_\ell^* = \frac{\#s_i \in (s_\ell^* - \Delta/2, s_\ell^* + \Delta/2)}{N}$$

- Typically, we pick L to be 1000, which is more than adequate

Steps for the Product Density ICA Algorithm

We can then approximate the objective function by:

$$\sum_{\ell=1}^L \left\{ y_{\ell}^* [\log(\phi(s_{\ell}^*)) + g(s_{\ell}^*)] - \Delta \phi(s_{\ell}^*) e^{g(s_{\ell}^*)} \right\} - \lambda \int g'''^2(s) ds$$

- ▶ can be seen to be proportional to a penalized Poisson log-likelihood with response y_{ℓ}^*/Δ and penalty parameter λ/Δ , and mean $\mu(s) = \phi(s)e^{g(s)}$
- ▶ a generalized additive spline model with an offset term $\log \phi(s)$ (Hastie and Tibshirani, 1990; Efron and Tibshirani, 1996)
- ▶ can be fit using a Newton algorithm