# LECTURE 6: Information Theory, Entropy, Experiment Design

- The concept of information theory and entropy appears in many statistical problems.
- Here we will develop some basic theory and show how it can be applied to questions such as how to compute statistical (in)dependence and how to design experiments such that we achieve the goals
- In principle the development mirrors classical statistical mechanics, but the is no corresponding concept of quantum statistics

# Information Theory

- Suppose we have a random variable with a discrete set of outcomes $p_i$, for $i$=1, ..., $M$
- We construct a message from $N$ independent outcomes of this variable
- We need $N\log_2 M$ bits to transmit this information
- But what if some are more likely than others: for large $N$ we expect $N_i = Np_i$ events for each $i$

# Information Theory

- Number of typical events is given by multinomial coefficient $g = N!/(\prod_{i=1}^{M} N_i!) << M^N$
- Remember Stirling formula $x! = x^x e^{-x}(2\pi x)^{1/2} + \ldots$
- The number of bits needed to specify one of g events in large $N$ limit is $log_2 g = -N\Sigma_i p_i log_2 p_i << Nlog_2 M$ : Shannon's theorem proves that in large N limit error with this number of bits vanishes
- Information content of $p$ is $I(p_i) = log_2 M + \Sigma_i p_i log_2 p_i$

# Entropy and information: discrete case

- Shannon information (Shannon 1948): *$h(x) = -log_2 p(x)$*
- Its average is called Shannon entropy: *$H(X)=-\Sigma_i p_i log_2 p_i$*
- $\log_2 g = \log_2 N!/(\Pi_{i=1}^{M} N_i!)$ is known as entropy of mixing in the context of mixing of M components
- Example: English alphabet has information content of 4.7+4.1 bit (p(x)=0: $0*\log_2 0=0$) ($\log_2 27=4.7$)
- Entropy is minimized at 0 for $p_i=\delta_{i,j}$ and maximized for $p_i=1/M$: it is a measure of disorder

| $i$ | $a_i$ | $p_i$ | $h(p_i)$ |
|---|---|---|---|
| 1 | a | .0575 | 4.1 |
| 2 | b | .0128 | 6.3 |
| 3 | c | .0263 | 5.2 |
| 4 | d | .0285 | 5.1 |
| 5 | e | .0913 | 3.5 |
| 6 | f | .0173 | 5.9 |
| 7 | g | .0133 | 6.2 |
| 8 | h | .0313 | 5.0 |
| 9 | i | .0599 | 4.1 |
| 10 | j | .0006 | 10.7 |
| 11 | k | .0084 | 6.9 |
| 12 | l | .0335 | 4.9 |
| 13 | m | .0235 | 5.4 |
| 14 | n | .0596 | 4.1 |
| 15 | o | .0689 | 3.9 |
| 16 | p | .0192 | 5.7 |
| 17 | q | .0008 | 10.3 |
| 18 | r | .0508 | 4.3 |
| 19 | s | .0567 | 4.1 |
| 20 | t | .0706 | 3.8 |
| 21 | u | .0334 | 4.9 |
| 22 | v | .0069 | 7.2 |
| 23 | w | .0119 | 6.4 |
| 24 | x | .0073 | 7.1 |
| 25 | y | .0164 | 5.9 |
| 26 | z | .0007 | 10.4 |
| 27 | - | .1928 | 2.4 |
| $\sum_i p_i \log_2 \frac{1}{p_i}$ | | | 4.1 |

# Relation between entropy and likelihood

- Instead of actual data likelihood we can replace it with its ensemble average
- Suppose we have $N$ measurements $x_i$

$$L = \prod_i p(x_i)$$

$$\ln L = \sum_i \ln p(x_i)$$

$$\left\langle \ln L \right\rangle = \left\langle \sum_i \ln p(x_i) \right\rangle = N \left\langle \ln p(X) \right\rangle$$

$$\left\langle \ln p(X) \right\rangle \text{ (or } E\{\ln p(X)\}) = \int dx \cdot p(X) \ln p(X) = -H(X)$$

$$\left\langle \ln L \right\rangle = -NH(X)$$

# Entropy for Continuous Distribution

$$H(X) = -\int p(x)\, log\, p(x) dx = E\{-log\, p(X)\}$$

- Not invariant under reparametrization: if we change $x$ to $F(x)$ entropy changes by $<|F'(x)|>$, so absolute value is meaningless. Not always positive definite. We will not distinguish $\log_2$ vs log/ln.
- In statistical mechanics this is solved by canonical conjugate pairs whose Jacobian is unity or if states are discretized (quantum statistics): no such concept in statistics

# Entropy for Continuous Distribution

- Joint entropy of X and Y

$$H(X,Y) = -\int p(x,y)\ log\ p(x,y)dx\ dy = E\{-log\ p(X,Y)\}$$

- Conditional entropy of X given y

$$H(X|y) = -\int p(x|y)\ log\ p(x|y)dx = E\{-log\ p(X|Y)\mid Y = y\}$$

- Conditional of X given Y

$$\begin{aligned} H(X|Y) &: \int p(y)H(X|y)dy = -\int p(y)\int p(x|y)\ log\ p(x|y)dxdy \\ &: -\int\int p(x,y)\ log\ p(x|y)dxdy = E\{E\{-log\ p(X|Y)\mid Y\}\} \end{aligned}$$

# Maximum Entropy

- For a bounded interval $a < x < b$ find $p$ with maximum entropy given the normalization constraint: use Lagrange multiplier method

$$H(p) \triangleq -\int_a^b p(x) \lg p(x)\, dx$$

$$\begin{aligned} p(x) &\geq 0 \\ \int_a^b p(x)\, dx &= 1. \end{aligned}$$

$$J(p) \triangleq -\int_a^b p(x) \ln p(x)\, dx + \lambda_0 \left( \int_a^b p(x)\, dx - 1 \right)$$

$$\frac{\partial}{\partial p(x)\, dx} J(p) = -\ln p(x) - 1 + \lambda_0.$$

$$p(x) = e^{\lambda_0 - 1}.$$

$$\lambda_0 = 1 - \ln(b - a)$$

$$p(x) = \begin{cases} \frac{1}{b-a}, & a \leq x \leq b \\ 0, & \text{otherwise.} \end{cases}$$

Uniform distribution maximizes entropy

# Maximum Entropy for Semi-unbounded Distributions

- If we are given mean on a semi-unbounded range from 0 to infinity, $p(x) = 0$ for $x < 0$

$$\int_{-\infty}^{\infty} x\, p(x)\, dx = \mu < \infty$$

$$\begin{aligned} J(p) \;\triangleq\; & -\int_0^{\infty} p(x) \ln p(x)\, dx + \lambda_0 \left( \int_0^{\infty} p(x)\, dx - 1 \right). \\ & + \lambda_1 \left( \int_0^{\infty} x\, p(x)\, dx - \mu \right) \end{aligned}$$

$$p(x) = \begin{cases} \frac{1}{\mu} e^{-x/\mu}, & x \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

Note the “Boltzmann” factor $e^{-\beta x}$

# Maximum Entropy for Unbounded Distributions

- If we are given mean $\mu$ and variance $s$ on an unbounded range from – to + infinity

$$
\begin{aligned}
J(p) &\triangleq -\int_{-\infty}^{\infty} p(x) \ln p(x)\, dx + \lambda_0 \left( \int_{-\infty}^{\infty} p(x)\, dx - 1 \right) \\
&+ \lambda_1 \left( \int_{-\infty}^{\infty} x\, p(x)\, dx - \mu \right) + \lambda_2 \left( \int_{-\infty}^{\infty} x^2\, p(x)\, dx - \sigma^2 \right)
\end{aligned}
$$

- $p(x) = e^{(\lambda_0 - 1) + \lambda_1 x + \lambda_2 x^2} = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}.$ if μ=0

- Can be further generalized: if we have constraints on first $n = 2k$ cumulants we obtain exponential of $n$-th order polynomial
- These "Boltzmann factors" have direct analogy with statistical mechanics

# Kullback-Leibler (KL) divergence

- KL divergence is a relative entropy between two distributions (discrete or continuous)

$$D_{\mathrm{KL}}(P\|Q)=\sum_i P(i)\,\log\frac{P(i)}{Q(i)}. \qquad D_{\mathrm{KL}}(P\|Q)=\int_{-\infty}^{\infty}p(x)\,\log\frac{p(x)}{q(x)}\,dx,$$

- Satisfies Gibbs inequality KL $\geq$ 0: proof using Jensen inequality for convex functions (see e.g. MacKay 2.7) or:

$$\ln x \leq x-1 \qquad -\sum_{i\in I}p_i\ln\frac{q_i}{p_i}\geq-\sum_{i\in I}p_i\left(\frac{q_i}{p_i}-1\right)$$
$$=-\sum_{i\in I}q_i+\sum_{i\in I}p_i$$

- This is 0 since probabilities are normalized
- It is not a distance: KL($p$,$q$) is not KL($q$,$p$)

# KL Divergence for Gaussians

- Always positive
- Increases as the two distributions differ from each other
- Only zero when the two distributions are equal
- Good way to probe how similar are two distributions: starting point for Variational Inference/Variational Bayes methods

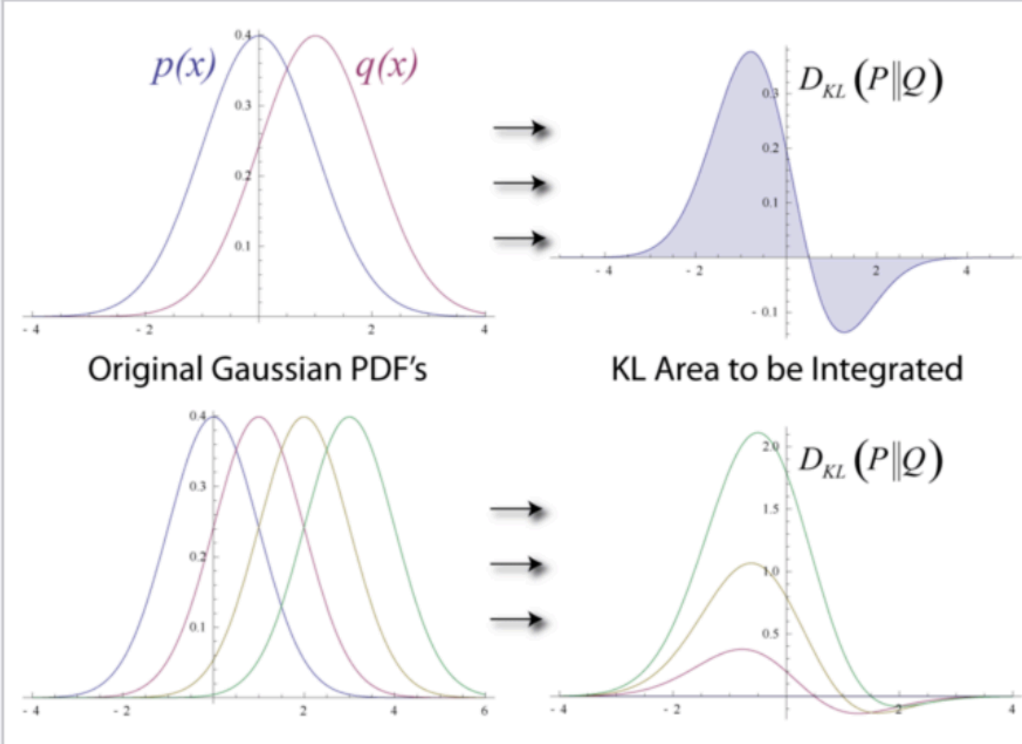



Illustration of the Kullback–Leibler (KL) divergence for two normal Gaussian distributions. Note the typical asymmetry for the Kullback–Leibler divergence is clearly visible.

# Exercise: KL Divergence for Gaussians

- Assume $p$ = gauss($\mu_1$, $\sigma_1$) and $q$ = gauss($\mu_2$, $\sigma_2$)
- Evaluate KL($p||q$) and show KL > 0
- Evaluate KL($q||p$) and show it differs from KL($p||q$)

# Solution: KL Divergence for Gaussians

$$KL(p||q) = \frac{1}{\sqrt{2\pi\sigma_1^2}} \int e^{\frac{-(x-\mu_1)^2}{2\sigma_1^2}} \Big[\frac{(x-\mu_2)^2}{2\sigma_2^2} - \frac{(x-\mu_1)^2}{2\sigma_1^2} + \frac{1}{2}\ln 2\pi(\sigma_2^2 - \sigma_1^2)\Big] dx$$

Let $u \equiv x - \mu_1, \;\; \Delta\mu = \mu_1 - \mu_2$

$$KL(p||q) = \frac{1}{\sqrt{2\pi\sigma_1^2}} \int e^{\frac{-u^2}{2\sigma_1^2}} \Big[\frac{(u-\Delta\mu)^2}{2\sigma_2^2} - \frac{u^2}{2\sigma_1^2} + \frac{1}{2}\ln 2\pi(\sigma_2^2 - \sigma_1^2)\Big] dx$$

$$= \frac{\sigma_1^2}{2\sigma_2^2} + \frac{\Delta\mu^2}{2\sigma_2^2} - \frac{1}{2} + \ln\sigma_2 - \ln\sigma_1$$

Minimized for $\Delta\mu = 0$

$$\frac{\sigma_1}{\sigma_2} = \alpha, \;\; \frac{\partial}{\partial\alpha}\Big(\frac{\alpha^2}{2} - \ln\alpha - \frac{1}{2}\Big) = 0, \;\; \alpha - \frac{1}{\alpha} = 0 \;\; \rightarrow \;\; \alpha = 1$$

Minimized for $\sigma_1 = \sigma_2$, KL = 0

$$KL(q||p) = \frac{\sigma_2^2}{2\sigma_1^2} + \frac{\Delta\mu^2}{2\sigma_1^2} - \frac{1}{2} + \ln\sigma_1 - \ln\sigma_2$$

# KL Divergence a and Negentropy

- Negentropy: KL divergence, i.e. relative entropy, against a Gaussian with equal variance

$$J(y) = H(y_G) - H(y) \geq 0$$

- Measures deviation of a distribution from gaussian. Can be approximated as

$$J(y) \approx \frac{1}{12} E\{y^3\}^2 + \frac{1}{48} kurt(y)^2$$

kurt($y$)=$E(y^4)$-3$E(y^2)^2$

- But other approximations may work better:

$$J(y) = [E\{G(y)\} - E\{G(g)\}]^2$$

$$G_1(y) = \frac{1}{a} log\ cosh\ (a\ y), \quad G_2(y) = -exp(-y^2/2)$$

# Mutual Information

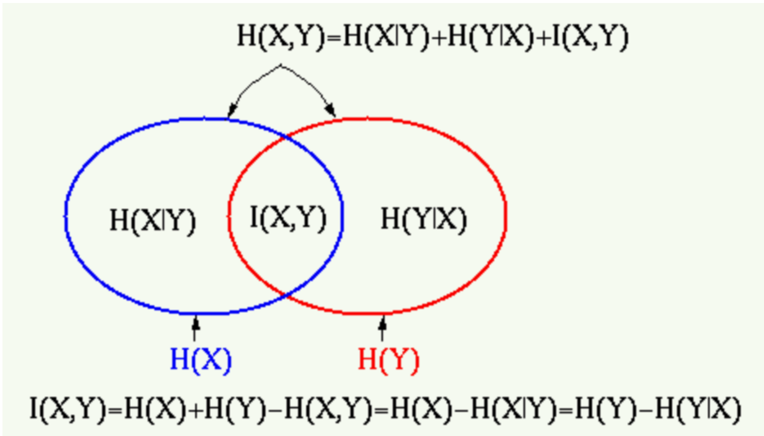
- Defined as amount of information shared between *X* and *Y*

$$I(X,Y) : H(X) + H(Y) - H(X,Y)$$
$$: E\{-log\ \ p(X)\} + E\{-log\ \ p(Y)\} + E\{-log\ \ p(X,Y)\}$$
$$: E\{log\ \frac{p(X,Y)}{p(X)\,p(Y)}\}$$

$$I(X,Y) : E\{log\ \frac{p(X,Y)}{p(X)\,p(Y)}\}$$
$$: E\{log\ \frac{p(X|Y)}{p(X)}\} = H(X) - H(X|Y)$$
$$: E\{log\ \frac{p(Y|X)}{p(Y)}\} = H(Y) - H(Y|X)$$

$$I(X;Y) = D_{\mathrm{KL}}(P(X,Y)\|P(X)P(Y))$$

- Minimizing $I(X,Y)$ is a good way to define independence: $I(X,Y)$=0 if $H(X|Y)$=$H(X)$ or $H(Y|X)$=$H(Y)$ and is positive (KL divergence)



# Multi-Information

- Generalization of mutual $I(\mathbf{y}) = \int P(\mathbf{y}) \log_2 \frac{P(\mathbf{y})}{\prod_i P(y_i)} d\mathbf{y}$
- Information $I(X,Y)$ to several variables $y$ (or $s$)
- Multi-information is 0 if $y$ statistically independent

$$I(\hat{\mathbf{s}}) = \sum_i H[(\mathbf{V}\mathbf{x}_w)_i] - H[\mathbf{V}\mathbf{x}_w]$$
$$= \sum_i H[(\mathbf{V}\mathbf{x}_w)_i] - (H[\mathbf{x}_w] + \log_2 |\mathbf{V}|)$$

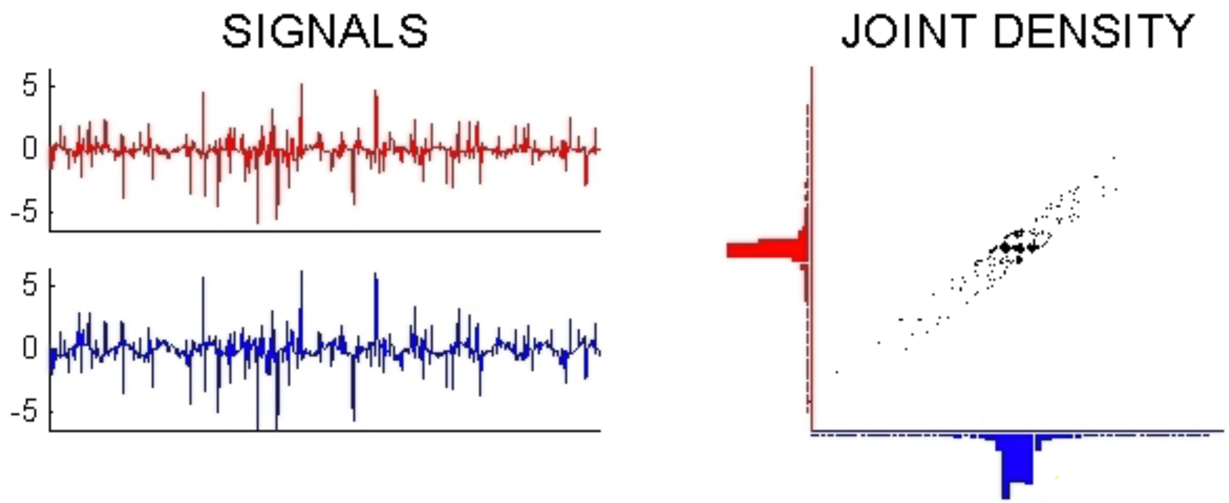
- ICA: we want to know V that minimizes $I(s)$, $s = Vx_w$

$$\mathbf{V} = \arg\min_{\mathbf{V}} \sum_i H[(\mathbf{V}\mathbf{x}_w)_i]$$

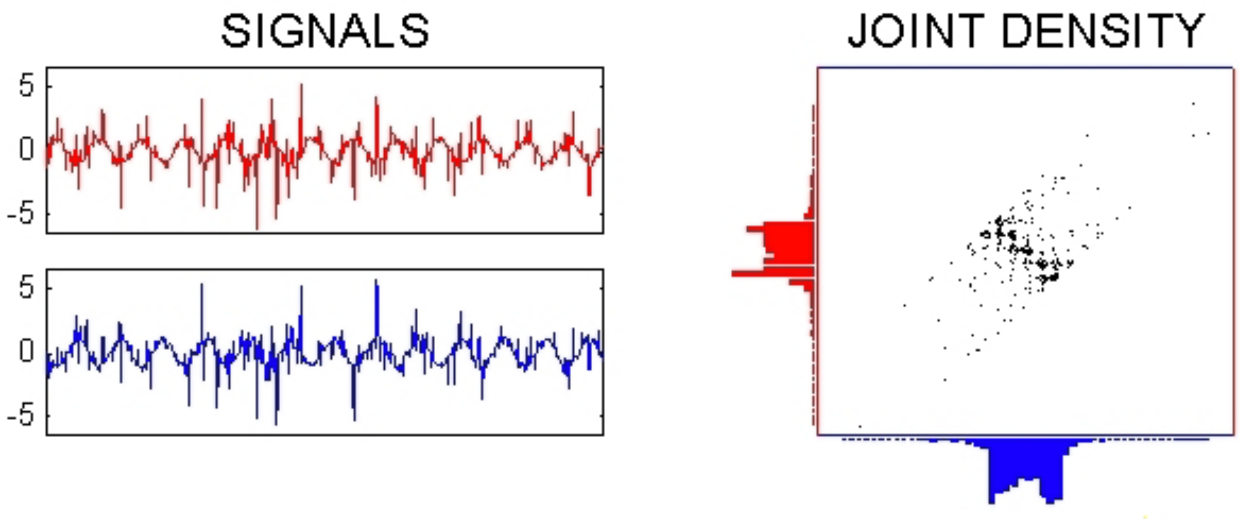
- This is equivalent to maximizing negentropy $J = \Sigma_\mathrm{i} [H(s_{gi})\text{-}H(s_i)]$ where $s = Vx_w$
- We do not know $P(s)$ so we need to use some approximation to evaluate relative entropy

# Fast ICA

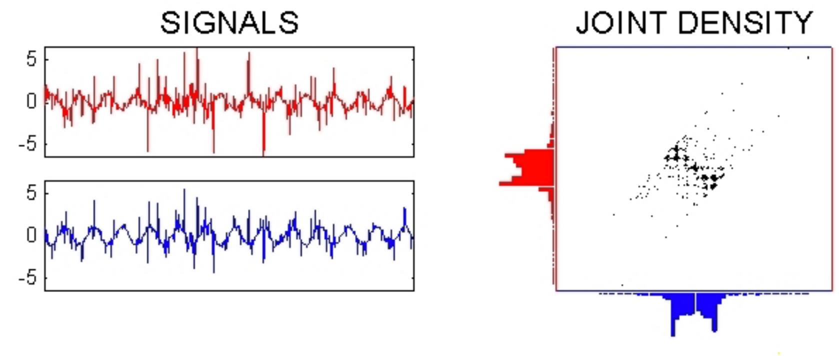
- Approximation for negentropy $J = [E(G(s))\text{-}E(G(g))]^2$
- Maximize $\Sigma_\mathrm{i} E(G(s_i)) = \Sigma_\mathrm{i} E(G(V^t_i x_w)) = E(G(V^t x_w))$
- Subject to normalization for $V$: Lagrange multiplier $\beta$
  $O(V) = E(G(V^t x_w))\text{-}\ \beta(V^T V\text{-}I)$
- This is optimization problem
- We will discuss how to solve optimization problems next, but typically this requires iterations, hence more complicated than linear algebra
- For large dimensions iterative methods are faster than linear algebra and even linear algebra problems are solved iteratively



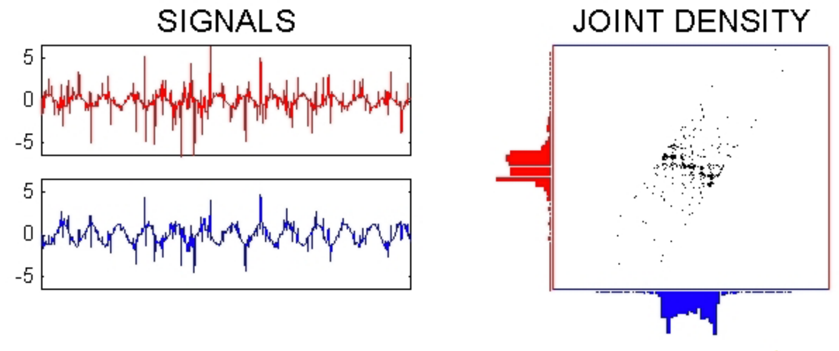

Input signals and density



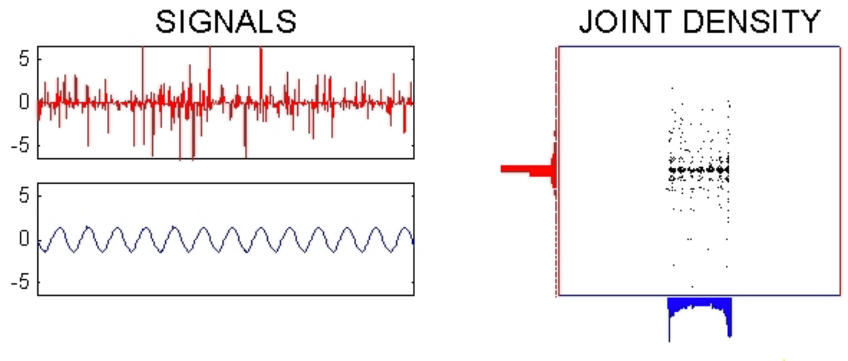

Whitened signals and density




**Separated signals after 1 step of FastICA**




**Separated signals after 2 steps of FastICA**




**Separated signals after 4 steps of FastICA**

Subsequent iterations rotate $V$ until it decorrelates the two signals

# Fisher Information Matrix (Metric)

- Quantify the power of future experiments
- Instead of actual data likelihood we can replace it with its ensemble average
- Suppose we have $N$ measurements $x_i$

$$L = \prod_i p(x_i)$$

$$\ln L = \sum_i \ln p(x_i)$$

$$\left\langle \ln L \right\rangle = \left\langle \sum_i \ln p(x_i) \right\rangle = N \left\langle \ln p(X) \right\rangle$$

$$\left\langle \ln p(X) \right\rangle \text{ (or } E\{\ln p(X)\}) = \int dx \cdot p(X) \ln p(X) = -H(X)$$

# Ensemble Averaging: Precision matrix becomes Fisher matrix.

- we can Taylor expand around a fiducial model in terms of parameters Θ we wish to measure

$$\ln L(\vec{\theta}_{\rm fid} + \Delta\vec{\theta}) = \ln L(\vec{\theta}_{\rm fid}) + \sum_i \frac{\partial \ln L}{\partial \theta_i}\Big|_{\vec{\theta}_{\rm fid}} \delta\theta_i + \frac{1}{2}\sum_{ij} \frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\Big|_{\vec{\theta}_{\rm fid}} \delta\theta_i \delta\theta_j$$

MLE: $\left\langle \frac{\partial \ln L}{\partial \theta_i} \right\rangle = E\left(\frac{\partial \ln p}{\partial \theta_i}\right) = 0$

Maximized at fiducial model: $\theta_i = \theta_{i,\rm fid}$

Fisher Matrix:

$$F_{ij} = -\left\langle \frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j} \right\rangle_{\theta_{\rm fid}} = \frac{\partial^2 H}{\partial\theta_i \partial\theta_j}$$

$$F_{ij} = \int dx \frac{\partial \ln p(x,\vec{\theta})}{\partial\theta_i} \frac{\partial \ln p(x,\vec{\theta})}{\partial\theta_j} p(x,\vec{\theta})$$

$$-\int p(x,\vec{\theta}dx = \int e^{-\ln p} dx = 1$$

$$\int e^{-\ln p} \frac{\partial \ln p}{\partial \theta_i} dx = 0$$

$$\int \left[ e^{-\ln p} \frac{\partial^2 \ln p}{\partial \theta_i \theta_j} - e^{-\ln p} \frac{\partial \ln p}{\partial \theta_i} \frac{\partial \ln p}{\partial \theta_j} \right] dx = 0$$

$$E\left(\frac{\partial^2 \ln p}{\partial \theta_i \theta_j}\right) = \int p \frac{\partial^2 \ln p}{\partial \theta_i \theta_j} dx = E\left(\frac{\partial \ln p}{\partial \theta_i} \frac{\partial \ln p}{\partial \theta_j}\right) = \int p \frac{\partial \ln p}{\partial \theta_i} \frac{\partial \ln p}{\partial \theta_j} dx$$

# Back to Linear Least Squares

$$-\ln L = \sum_i \frac{\left(y_i - y(x_i|\vec{\theta})\right)^2}{2\sigma_i^2}$$

$$\left\langle \frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j} \right\rangle = \left\langle \sum_k \frac{\frac{\partial y(x_k)}{\partial\theta_i}\frac{\partial y(x_k)}{\partial\theta_j}}{2\sigma_i^2} \right\rangle = F_{ij}$$

Posterior: $p(\vec{\theta}) \;\propto\; e^{-\delta\theta_i F_{ij}\delta\theta_j/2}$

Covariance Matrix: $\left\langle \theta_i \theta_j \right\rangle = \left\langle \theta_i \right\rangle \left\langle \theta_j \right\rangle = F_{ij}^{-1}$

# Experiment Design

- When we design an experiment we may be able to choose several parameters: sampling of points $x_i$ where we measure data $y_i$, noise level $\sigma_i$, number of data points $x_i$ etc.
- At a given $\mathrm{x_i}$ information on parameter $\Theta_j$ is given by $(dy_i/d\Theta_j)^2/\sigma_i^2$: this suggests choosing $x_i$ where this is maximized. Note that this can be computed at the fiducial model without actually taking any data
- If we have several parameters we need to break their degeneracies: this is not possible if we only observe at a single $x_i$: we need to compute full Fisher matrix and invert it to obtain the final error estimate
- By varying the design of the experiment we can predict what the expected error on any given parameter will be: this enables us to design experiment to reach the goals we wish to achieve

# Literature

- D. Mackay, *Information Theory, Inference, and Learning Algorithms* (See course website), Chapter 2
- M. Kardar, *Statistical Physics of Particles*, Chapter 2
- ICA: J. Shlens, *A Tutorial on Independent Component Analysis*, https://arxiv.org/pdf/1404.2986.pdf