Spectrum of random correlation matrices

$$X_{ia} = x_i^a \quad , \quad \text{with } x = \mathcal{N}(0, \sigma^2 = 1)$$

$a = 1 \ldots P$ observations

$i = 1 \ldots N$ variables

Correlation matrix (this is a Wishart matrix!)
$$C_{ij} = \frac{1}{P} \sum_{a=1}^{P} x_i^a x_j^a = \frac{1}{P}(X X^T)_{ij}$$

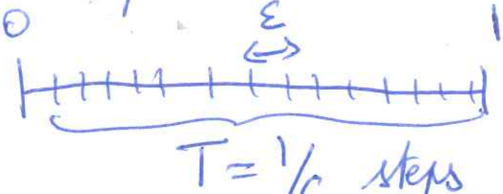
Parameter : $r = \frac{N}{P}$ = "noise" level

* $r \to 0$ means perfect sampling: $C_{ij} = \delta_{ij}$
* we assume hereafter that $r < 1$.
  Case $r > 1$ is similar, except that there are $(1 - \frac{1}{r}) N = N - P$ null eigenvalues since $\mathrm{rank}(C) \leq \min(N, P)$

We want to compute the spectrum of C:
$$C |u\rangle^\alpha = \lambda^\alpha |u\rangle^\alpha \quad , \quad \alpha = 1 \ldots N$$

<u>Idea</u>: we invent a dynamical process to create the data X

Variance of x:



$$x_i^a = \sum_{t=1}^{T} \delta x_i^a(t) \;, \quad \text{with } \delta x_i^a(t) = \mathcal{N}(0, \sigma^2 = \varepsilon)$$

Indeed:
$$\overline{x_i^a} = T \cdot \overline{\delta x_i^a(t)} = \frac{1}{\varepsilon} \cdot 0 = 0$$
$$\overline{(x_i^a)^2} = T \cdot \overline{\delta x_i^a(t)^2} = \frac{1}{\varepsilon} \cdot \varepsilon = 1$$
(any t)

and, obviously, $\overline{\delta x_i^a(t)\, \delta x_j^a(t')} = 0$ if $i \neq j, t \neq t'$

Calculation : we will track the dynamics of the eigenvalues of C as time evolves.

- Initially $(t=0)$: $C=0$, hence $\lambda^\alpha = 0 \ \forall \alpha$
- What happens between t and $t+\varepsilon$?

$$X \to X + \delta X \Rightarrow C = C + \delta C \quad \text{with}$$

$$\delta C = \underbrace{\frac{1}{P}\left(\delta X . X^T + X . \delta X^T\right)}_{1^{st} \text{ order in } \delta X} + \underbrace{\frac{1}{P}\left(\delta X . \delta X^T\right)}_{2^{nd} \text{ order in } \delta X}$$

- Perturbation theory (same as in Quantum Mechanics ...)

$$\delta\lambda^\alpha = \underbrace{\langle u^\alpha | \delta C | u^\alpha \rangle}_{1^{st} \text{ order in } \delta C} + \underbrace{\sum_{\beta(\neq\alpha)} \frac{|\langle u^\beta | \delta C | u^\alpha \rangle|^2}{\lambda^\alpha - \lambda^\beta}}_{2^{nd} \text{ order in } \delta C} + \dots$$

$$* \ \overline{\langle u^\alpha | \delta C | u^\alpha \rangle} = \langle u^\alpha | \frac{1}{P} \overline{(\delta X . \delta X^T)} | u^\alpha \rangle \quad \text{since } \overline{\delta X} = 0 = \overline{\delta X^T}$$

$$= \frac{1}{P} \sum_{ij} u_i^\alpha u_j^\alpha \left(\overline{\sum_a \delta x_i^a \delta x_j^a} \right)$$

$$\text{“} P . \varepsilon \delta_{ij} \text{”}$$

$$= \varepsilon \left(\sum_i u_i^\alpha\right)^2 = \varepsilon$$

$$* \ \overline{\underbrace{\langle u^\beta | \delta C | u^\alpha \rangle}_{\text{real number}}{}^2} \underset{\substack{\text{(we neglect} \\ \delta X . \delta X^T \text{ to} \\ \text{this order)}}}{\simeq} \frac{1}{P^2} \overline{\langle u^\beta | (\delta X . X^T + X . \delta X^T) | u^\alpha \rangle^2}$$

$$= \frac{1}{P^2} \sum_{\substack{ij \\ i'j'}} u_i^\beta u_j^\alpha u_{i'}^\beta u_{j'}^\alpha \sum_{aa'} \overline{\left(\delta x_i^a x_j^a + x_i^a \delta x_j^a\right)\left(\delta x_{i'}^{a'} x_{j'}^{a'} + x_{i'}^{a'} \delta x_{j'}^{a'}\right)}$$

$$\overline{(-+-)(-+-)} = \varepsilon\, \delta_{ii'}\, \delta^{aa'}\, x_j^a x_{j'}^{a'} + \varepsilon\, \delta_{ij'}\, \delta^{aa'}\, x_j^a x_{i'}^{a'} + \varepsilon\, \delta_{ji'}\, \delta^{aa'}\, x_i^a x_{j'}^{a'} + \varepsilon\, \delta_{jj'}\, \delta^{aa'}\, x_i^a x_{i'}^{a'}$$

Each δ leads to the computation of the overlap between u and u:

<u>example</u>:

$$\delta_{ii'} \longrightarrow \sum_i u_i^\beta u_{i'}^\beta \delta_{ii'} = 1$$

$$\delta_{ij'} \longrightarrow \sum_{ij'} u_i^\beta u_{j'}^\alpha \delta_{ij'} = \langle u^\beta | u^\alpha \rangle = 0$$

similarly: $\delta_{jj'} \to 1$, $\delta_{ji'} \to 0$

<u>Hence:</u>

$$\overline{\langle u^\beta | \delta C | u^\alpha \rangle^2} = \frac{\varepsilon}{P^2}\left(\sum_{jj'} \underbrace{\sum_a x_j^a x_{j'}^a}_{P.\,C_{jj'}} u_j^\alpha u_{j'}^\alpha + \sum_{ii'} \underbrace{\sum_a x_i^a x_{i'}^a}_{P.\,C_{ii'}} u_i^\beta u_{i'}^\beta \right)$$

$\delta_{ii'}$ term $\qquad \delta_{jj'}$ term

$$= \frac{\varepsilon}{P}\left(\langle u^\alpha | C | u^\alpha \rangle + \langle u^\beta | C | u^\beta \rangle \right)$$

$$= \frac{\varepsilon}{P}\left(\lambda^\alpha + \lambda^\beta \right)$$

On average, we get:

$$\delta\lambda^\alpha = \varepsilon \cdot \left(1 + \frac{1}{P} \sum_{\beta (\neq \alpha)} \frac{\lambda^\alpha + \lambda^\beta}{\lambda^\alpha - \lambda^\beta} \right) \qquad \lambda^\beta = \lambda^\beta - \lambda^\alpha + \lambda^\alpha$$

$$= \varepsilon \left(1 + \frac{2\lambda^\alpha}{P} \sum_{\beta(\neq\alpha)} \frac{1}{\lambda^\alpha - \lambda^\beta} - \frac{N-1}{P} \right)$$

$\simeq r$ for large N, P.

Continuous time: $\lambda^\alpha(t+\varepsilon) = \lambda^\alpha(t) + \delta\lambda^\alpha$

$$\Rightarrow \lambda^\alpha(t) + \varepsilon \frac{d\lambda^\alpha}{dt} = \lambda^\alpha(t) + \delta\lambda^\alpha \Rightarrow \boxed{\frac{d\lambda^\alpha}{dt} = 1 - r + \frac{2\lambda^\alpha}{N} \sum_{\beta(\neq\alpha)} \frac{1}{\lambda^\alpha - \lambda^\beta}}$$

<u>One remark:</u> deviation from the average can be computed, they vanish as $\frac{1}{\sqrt{N}}$ for large N; hence dynamics of spectrum eigenvalues becomes deterministic.

We need to solve N ODE; to do so we introduce the generating function:

$$G(z,t) = \frac{1}{N}\sum_{\alpha=1}^{N} \frac{1}{z-\lambda^{\alpha}(t)}$$

(called Stieljes transform)

(quite natural from the structure of ODE)

Then, we write the N coupled ODEs as a single PDE for G:

$$\frac{\partial G}{\partial t} = \frac{1}{N}\sum_{\alpha} \frac{1}{(z-\lambda^{\alpha})^2}\,\underbrace{\frac{d\lambda^{\alpha}}{dt}}_{\substack{\shortparallel \\ 1-r+2r\underbrace{\lambda^{\alpha}}_{\lambda^{\alpha}-z+z}\frac{1}{N}\sum_{\beta(\neq\alpha)}\frac{1}{\lambda^{\alpha}-\lambda^{\beta}}}}$$

$$= \frac{1}{N}\sum_{\alpha}\left\{\frac{1}{(z-\lambda^{\alpha})^2}\left(1-r+2rz\frac{1}{N}\sum_{\beta(\neq\alpha)}\frac{1}{\lambda^{\alpha}-\lambda^{\beta}}\right) - \frac{2r}{z-\lambda^{\alpha}}\frac{1}{N}\sum_{\beta(\neq\alpha)}\frac{1}{\lambda^{\alpha}-\lambda^{\beta}}\right\}$$

$$= \frac{\partial}{\partial z}\left\{\frac{1}{N}\sum_{\alpha}\frac{1}{z-\lambda^{\alpha}}\left(-1+r-\frac{2rz}{N}\sum_{\beta(\neq\alpha)}\frac{1}{\lambda^{\alpha}-\lambda^{\beta}}\right)\right\}$$

$$= -(1-r)\frac{\partial}{\partial z}G - 2r\frac{\partial}{\partial z}\left(z\cdot\frac{1}{N^2}\sum_{\alpha\neq\beta}\frac{1}{(z-\lambda^{\alpha})(\lambda^{\alpha}-\lambda^{\beta})}\right)$$

<u>Note:</u> $\sum_{\alpha\neq\beta} A_{\alpha\beta} = \sum_{\alpha\neq\beta} A_{\beta\alpha}$

$$= \frac{1}{2}\sum_{\alpha\neq\beta}\left(A_{\alpha\beta}+A_{\beta\alpha}\right)$$

Here, $A_{\alpha\beta} = \frac{1}{(z-\lambda^{\alpha})(\lambda^{\alpha}-\lambda^{\beta})} \Rightarrow \frac{1}{2}(A_{\alpha\beta}+A_{\beta\alpha}) = \frac{1}{2}\left(\frac{1}{(z-\lambda^{\alpha})}-\frac{1}{(z-\lambda^{\beta})}\right)\cdot\frac{1}{\lambda^{\alpha}-\lambda^{\beta}}$

$$= \frac{\lambda^{\alpha}-\lambda^{\beta}}{(z-\lambda^{\alpha})(z-\lambda^{\beta})}$$

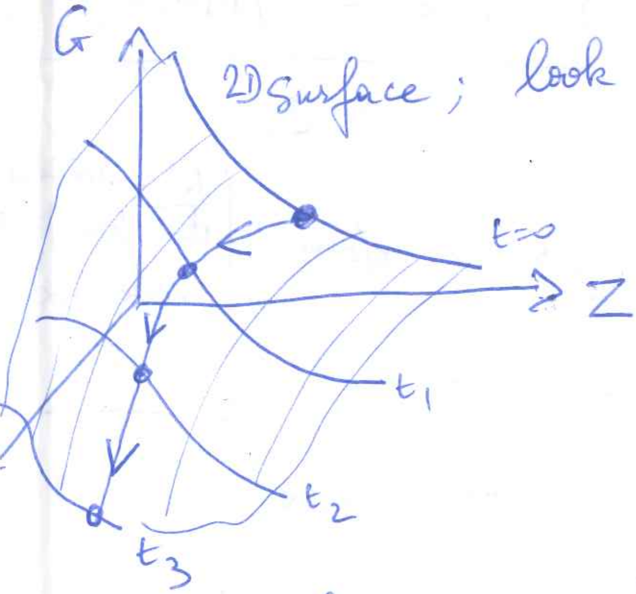
Hence,

$$\frac{\partial G}{\partial t} = -(1-r)\frac{\partial G}{\partial z} - 2r\frac{\partial}{\partial z}\Bigg(\underbrace{\frac{z}{2N^2}\sum_{\alpha\neq\beta}\frac{1}{(z-\lambda^\alpha)(z-\lambda^\beta)}}_{\xrightarrow[N\to\infty]{} z\cdot\frac{1}{2}G(z,t)^2}\Bigg)$$

$$\boxed{\frac{\partial G}{\partial t} + \left(1-r+2rzG\right)\frac{\partial G}{\partial z} + rG^2 = 0}$$

initial condition : $\quad G(z,t=0) = \dfrac{1}{z}$.

Methods of Characteristics :



2D surface ; look for trajectory $z(t), g(t) = G(z(t),t)$ starting in $(z_0, g_0 = \frac{1}{z_0})$

$$\dot{g} = \frac{\partial G}{\partial z}\dot{z} + \frac{\partial G}{\partial t}$$
$$= -rg^2 + \frac{\partial G}{\partial z}\left(\dot{z} - (1-r+2rzg)\right)$$

So we choose :
$$\begin{cases} \dot{z} = 1-r+2rzg & (1) \\ \dot{g} = -rg^2 & (2) \end{cases}$$

(2) gives $\quad g(t) = \dfrac{1}{z_0+rt}$, then insert g in (1)

(1) gives $\quad z(t) = \left(t+\dfrac{z_0}{r}\right)\left(\dfrac{rt}{z_0}+r\right)$
$$= (z_0+rt)\left(1+\frac{t}{z_0}\right)$$

We eliminate z_0 : $z_0 = \frac{1}{g} - rt$, to get:

$$z = \left(\frac{1}{g} - rt + rt\right)\left(1 + t\left(\frac{1}{g} - rt\right)^{-1}\right)$$

i.e. $$z = \frac{1}{g} + \frac{t}{1 - rtg}$$

We now express g as a function of z:

$$g = G(z,t) = \frac{z + (r-1)t \pm \sqrt{z^2 - 2zt(1+r) + t^2(1-r)^2}}{2rtz}$$

We have to choose the "$-$" sign to match $\frac{1}{z}$ in $t=0$.

<u>Hence:</u>

$$\boxed{G(z, t=1) = \frac{z + r - 1 - \sqrt{z^2 - 2z(1+r) + (1-r)^2}}{2rz}}$$

NB: remark that $G(z,t) = \frac{1}{t} g\left(\frac{z}{t}\right)$ since $\lambda \propto t$

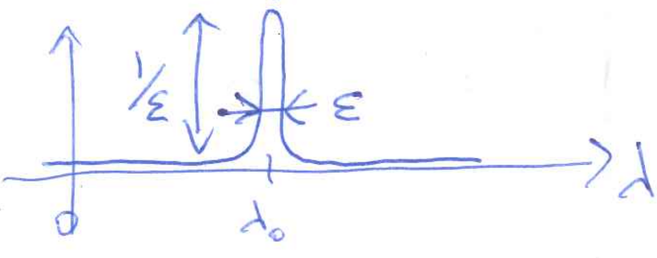
We now need to invert the Stieltjes transform:

$$G(z) = \frac{1}{N} \sum_\alpha \frac{1}{z - \lambda^\alpha} \underset{N \to \infty}{=} \int_0^\infty d\lambda \, \frac{\rho(\lambda)}{z - \lambda}$$

This can be easily done with a bit of complex analysis:

$$G(\underset{\text{real}}{\lambda_0} + i\varepsilon) = \int_0^\infty d\lambda \, \frac{\rho(\lambda)}{\lambda_0 - \lambda + i\varepsilon} = \int_0^\infty d\lambda \, \frac{\rho(\lambda)}{(\lambda_0 - \lambda)^2 + \varepsilon^2} (\lambda_0 - \lambda - i\varepsilon)$$

$$\Rightarrow -\text{Im}\, G(\lambda_0 + i\varepsilon) = \int_0^\infty d\lambda \, \rho(\lambda) \times \frac{\varepsilon}{(\lambda_0 - \lambda)^2 + \varepsilon^2}$$

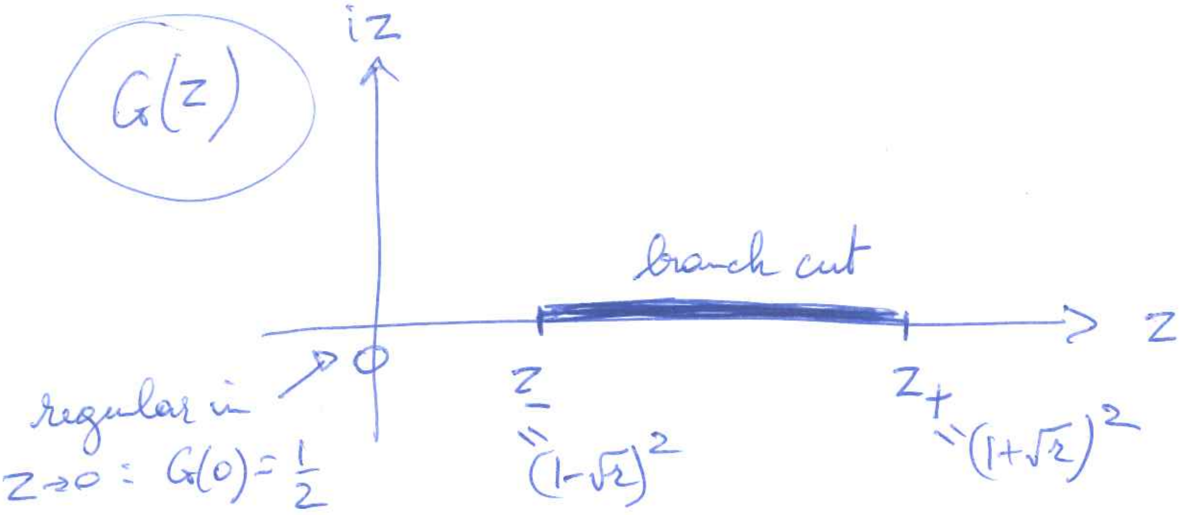


change of variable : $\lambda = \lambda_0 + u\varepsilon$:

$$-\text{Im}\, G(\lambda_0 + i\varepsilon) = \int_{-\lambda_0/\varepsilon}^{\infty} du.\, \varepsilon \rho(\lambda_0 + u\varepsilon) \cdot \frac{\varepsilon}{(u^2+1)\varepsilon^2}$$

$$\xrightarrow[\varepsilon \to 0]{} \rho(\lambda_0) \cdot \underbrace{\int_{-\infty}^{+\infty} \frac{du}{1+u^2}}_{=\pi}$$

$$\Rightarrow \quad \boxed{\rho(\lambda) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \text{Im}\left(G(\lambda + i\varepsilon)\right)}$$



$z_\pm$ such that $z^2 - 2z(1+r) + (1-r)^2 = 0$

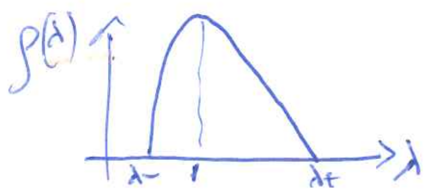
i.e. $z_\pm = (1 \pm \sqrt{r})^2$

For $\lambda < z_-$ or $\lambda > z_+$: $\text{Im}\, G(\lambda + i\varepsilon) \xrightarrow[\varepsilon \to 0^+]{} 0$

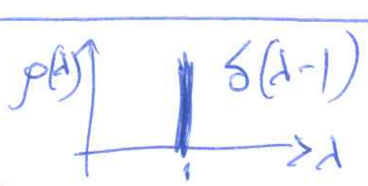
For $z_- < \lambda < z_+$: $\text{Im}\, G(\lambda + i\varepsilon) = -\frac{1}{2r\lambda}\sqrt{(z_+ - \lambda)(\lambda - z_-)}$

Marcenko Pastur distribution

$$\boxed{\rho(\lambda) = \frac{\sqrt{(\lambda_+ - \lambda)(\lambda - \lambda_-)}}{2\pi r \lambda}}$$



$\xrightarrow[r \to 0]{}$



NB: distribution is universal, i.e. holds for non Gaussian i.i.d. variables

The spiked covariance model and the phase transition

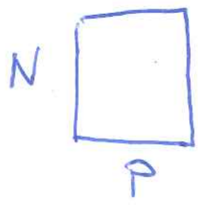
We consider the case of correlated random variables, i.e. the covariance of the Gaussian distribution is

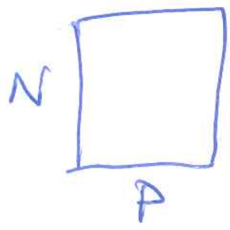
$$\underset{\substack{\uparrow \\ N\times N \text{ identity matrix}}}{\Sigma \neq I} \quad , \quad \text{e.g. } \Sigma = I + s\,|e\rangle\langle e| \ \text{ with } s>0.$$

This is one the simplest correlated model one can think of, called spiked covariance model.

The covariance matrix for P observations is:

$$C' = \frac{1}{P}\, Y \cdot Y^T \quad , \quad \text{with} \quad Y = \Sigma^{1/2} \cdot \underset{\substack{\uparrow \\ \text{uncorrelated data matrix}}}{X}$$





Spectrum of C' = Spectrum of $P^{-1} C' P$ for any change of basis P

$$\underset{P = \Sigma^{-1/2}}{=} \text{Spectrum of } \underbrace{\Sigma^{-1/2}\left(\Sigma^{1/2} X X^T \Sigma^{1/2}\right)\Sigma^{1/2}}_{C.\Sigma}$$

C: Marcenko Pastur matrix (called Wishart matrix, 1926)

$z \in$ Spectrum of $C' \iff \det(zI - C\Sigma) = 0$

$\iff \det\left(zI - C - s\, C|e\rangle\langle e|\right) = 0$

Either $z \in$ Spectrum of C or $M(z) = zI - C$ is invertible, and we have

$$\underbrace{\det M(z)}_{\substack{\neq \\ 0 \text{ by hypothesis}}} \times \det\left(I - s\,\underbrace{M(z)^{-1} C\,|e\rangle\langle e|}_{\text{hence, rank one matrix, with:}}\right) = 0.$$

hence, rank one matrix, with:
* $N-1$ eigenvalues $= 0$
* 1 eigenvalue $= 1$

This is equivalent to saying that the trace of this rank one matrix is equal to one:

$$\langle e|\frac{C}{zI - C}|e\rangle = \frac{1}{s}$$

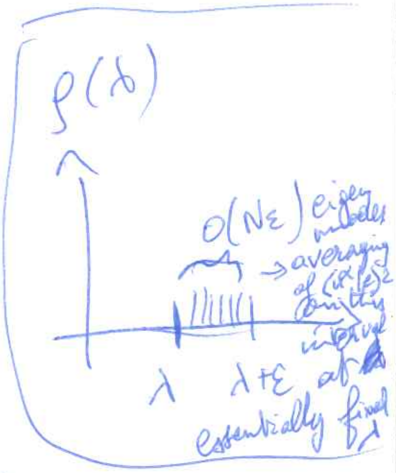
Let $\lambda^\alpha, |u^\alpha\rangle$ be the eigenvalues, eigenmodes of C:

$$\sum_{\alpha=1}^{N} \frac{\lambda^\alpha}{z - \lambda^\alpha} \langle e|u^\alpha\rangle^2 = \frac{1}{s}$$

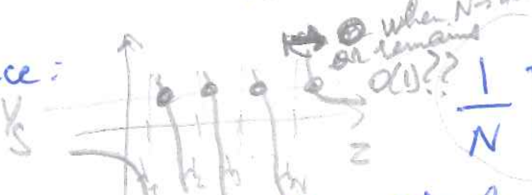
As $|e\rangle$ and the $|u_\alpha\rangle$ are totally uncorrelated, on average over C, we expect:

$$\langle e|u^\alpha\rangle^2 = \frac{1}{N}$$

since $\sum_{\alpha=1}^{N} \langle e|u^\alpha\rangle^2 = \langle e|e\rangle = 1.$



Hence:



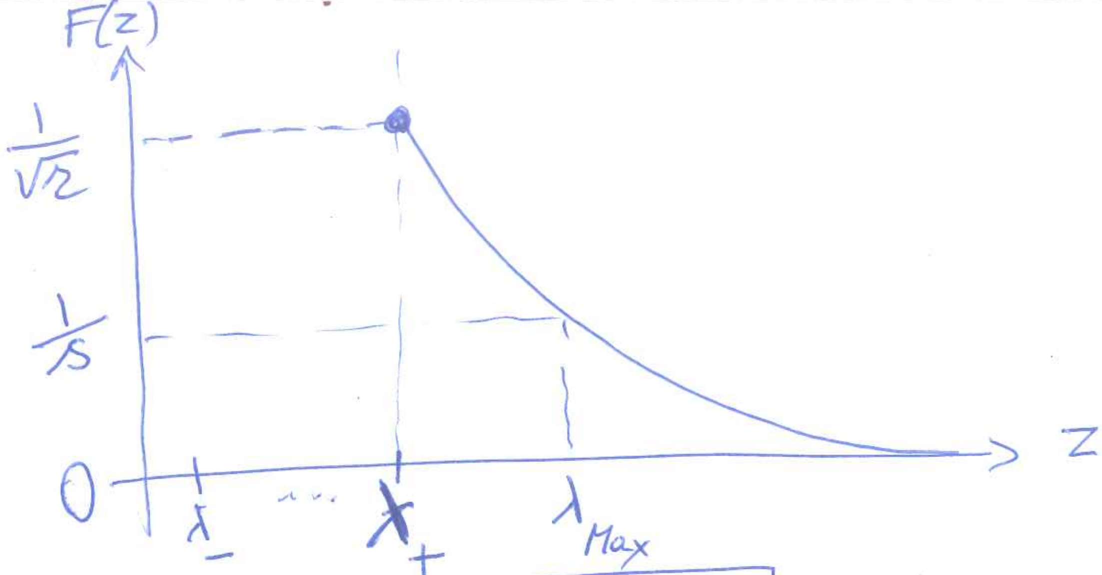
$$\frac{1}{N}\sum_{\alpha=1}^{N} \frac{\lambda^\alpha}{z - \lambda^\alpha} = \frac{1}{s}$$

We recognize the Stieltjes transform of $\rho(\lambda)$:

$$\frac{1}{s} = \int_{\lambda_-}^{\lambda_+} d\lambda\, \rho(\lambda)\, \frac{\lambda}{z-\lambda} = \int_{\lambda_-}^{\lambda_+} d\lambda\, \rho(\lambda)\, \frac{\lambda - z + z}{z - \lambda} = z\,G(z) - 1$$

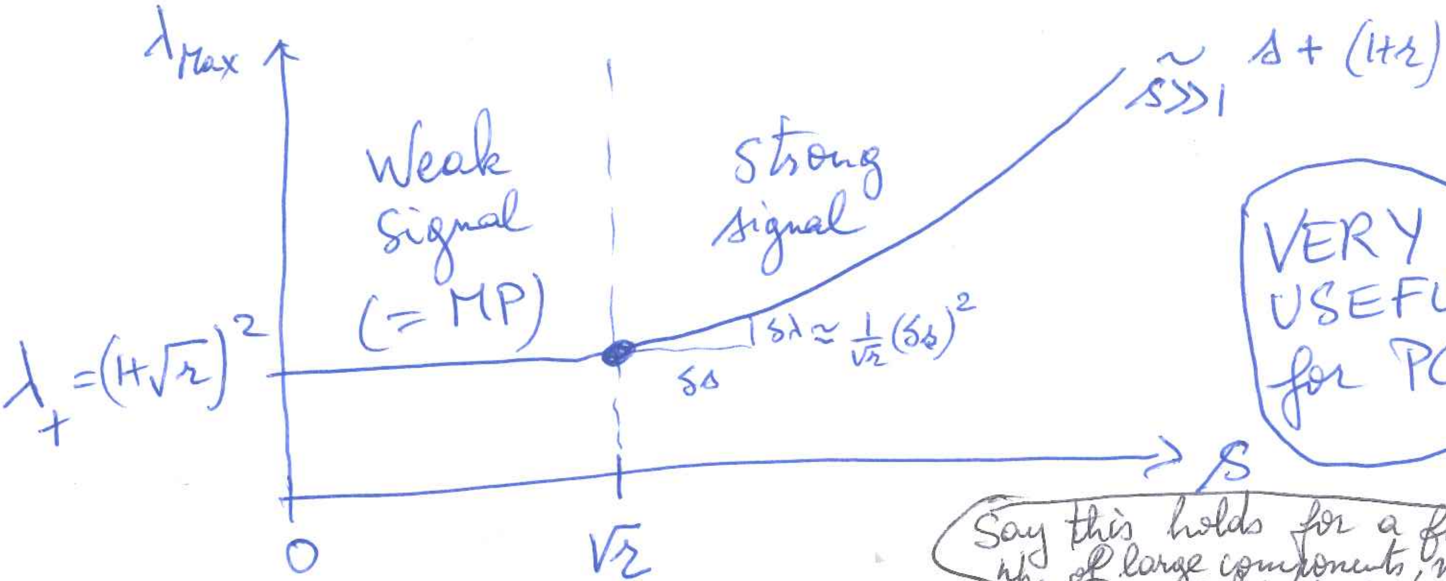
Hence, using the previous expression for G:

$$\boxed{\frac{1}{s} = \frac{1}{2r}\left(z - r - 1 - \sqrt{z^2 - 2z(1+r) + (1-r)^2}\right)} \equiv F(z)$$



There is a solution if $\boxed{s > \sqrt{r}}$; $\lambda_{Max} = 1 + r + s + \frac{r}{s}$

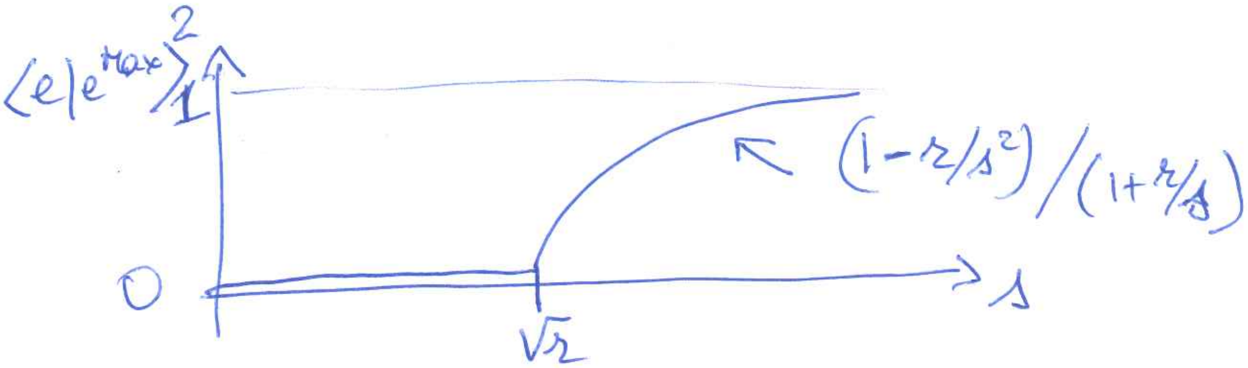
This is the signature of a phase transition:



VERY USEFUL for PCA!

Say this holds for a finite nb. of large components, not only one

One can show that $|e^{Max}\rangle$, associated to λ^{Max}, is "aligned" along $|e\rangle$ in the strong signal phase:



can be pushed ← to the left by using priors on $|e\rangle$, e.g. potential on the components, $P_0(|e\rangle) = \cancel{\simeq} \left(\frac{\gamma}{2}\right)^N e^{-\gamma \sum_i |e_i|}$