part I of a short course on

The replica method and its applications in biomedical modelling and data analysis

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replica method

A clever trick that enables the analytical calculation of averages that are normally impossible to do, except numerically.

is particularly useful for

Complex heterogeneous systems composed of *many* interacting variables, and with *many* parameters on which we have only statistical information. (too large for numerical averages to be computationally feasible)

gives us

Analytical predictions for the behaviour of *macroscopic* quantities in *typical* realisations of the systems under study.

note on biomedical applications

The 'large systems' could describe actual *biochemical processes* (folding proteins, proteome, transcriptome, immune or neural networks, etc), or *analysis algorithms* running on large biomedical data sets

1. Mathematical preliminaries
   - The delta distribution
   - Gaussian integrals
   - Steepest descent integration
2. The replica method
   - Exponential families and generating functions
   - The replica trick
   - The replica trick and algorithms
   - Alternative forms of the replica identity
3. Application: information storage in neural networks
   - Attractor neural networks
   - The replica calculation
   - Replica symmetry
   - Replica symmetric solution
4. Application: overfitting transition in linear separators
   - Linear separability of data – version space
   - The replica calculation
   - Gardner's replica symmetric theory
   - Overfitting transition in Cox regression

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The δ-distribution

- **intuitive definition** of $\delta(x)$:

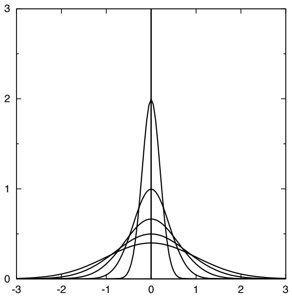
  prob distribution for a 'random' variable x
  that is always zero

  $$\langle f\rangle=\int_{-\infty}^{\infty}\mathrm{d}x\ f(x)\delta(x)=f(0) \qquad \textit{for any } f$$

  for instance

  $$\delta(x)=\lim_{\sigma\to 0}\frac{1}{\sigma\sqrt{2\pi}}\,e^{-x^2/2\sigma^2}$$

  not a function: $\delta(x\neq 0)=0,\ \ \delta(0)=\infty$



- status of $\delta(x)$:

  $\delta(x)$ only has a meaning when appearing *inside an integration*,
  one takes the limit $\sigma\!\downarrow\!0$ *after* performing the integration

$$\int_{-\infty}^{\infty}\mathrm{d}x\ f(x)\delta(x)=\lim_{\sigma\downarrow 0}\int_{-\infty}^{\infty}\mathrm{d}x\ f(x)\frac{e^{-x^2/2\sigma^2}}{\sigma\sqrt{2\pi}}=\lim_{\sigma\downarrow 0}\int_{-\infty}^{\infty}\mathrm{d}x\ f(x\sigma)\frac{e^{-x^2/2}}{\sqrt{2\pi}}=f(0)$$

- **differentiation** of $\delta(x)$:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, f(x)\delta'(x) = \int_{-\infty}^{\infty} \mathrm{d}x \left\{ \frac{\mathrm{d}}{\mathrm{d}x}\Big(f(x)\delta(x)\Big) - f'(x)\delta(x) \right\}$$

$$= \lim_{\sigma\downarrow 0} \left[f(x) \frac{e^{-x^2/2\sigma^2}}{\sigma\sqrt{2\pi}} \right]_{x=-\infty}^{x=\infty} - f'(0) = -f'(0)$$

generalization:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \frac{\mathrm{d}^n}{\mathrm{d}x^n}\delta(x) = (-1)^n \lim_{x\to 0} \frac{\mathrm{d}^n}{\mathrm{d}x^n} f(x) \qquad (n = 0, 1, 2, \ldots)$$

- **integration** of $\delta(x)$:

$$\delta(x) = \frac{\mathrm{d}}{\mathrm{d}x}\theta(x) \qquad \begin{array}{l} \theta(x<0) = 0 \\ \theta(x>0) = 1 \end{array}$$

Proof: both sides have same effect in integrals

$$\int \mathrm{d}x \left\{ \delta(x) - \frac{\mathrm{d}}{\mathrm{d}x}\theta(x) \right\} f(x) = f(0) - \lim_{\epsilon\downarrow 0} \int_{-\epsilon}^{\epsilon} \mathrm{d}x \left\{ \frac{\mathrm{d}}{\mathrm{d}x}\Big(\theta(x)f(x)\Big) - f'(x)\theta(x) \right\}$$

$$= f(0) - \lim_{\epsilon\downarrow 0} [f(\epsilon) - 0] + \lim_{\epsilon\downarrow 0} \int_0^{\epsilon} \mathrm{d}x\, f'(x) = 0$$

- **generalization** to vector arguments:

$$\mathbf{x} \in \mathbb{R}^N: \qquad \delta(\mathbf{x}) = \prod_{i=1}^{N} \delta(x_i)$$

- **Integral representation** of $\delta(x)$

  use defns of Fourier transforms and their inverse:

$$\hat{f}(k) = \int_{-\infty}^{\infty} \mathrm{d}x\; e^{-2\pi \mathrm{i} kx} f(x) \qquad f(x) = \int_{-\infty}^{\infty} \mathrm{d}k\; e^{2\pi \mathrm{i} kx} \hat{f}(k) \quad \Rightarrow \quad f(x) = \int_{-\infty}^{\infty} \mathrm{d}k\; e^{2\pi \mathrm{i} kx} \int_{-\infty}^{\infty} \mathrm{d}y\; e^{-2\pi \mathrm{i} ky} f(y)$$

  apply to $\delta(x)$: $\quad \delta(x) = \int_{-\infty}^{\infty} \mathrm{d}k\; e^{2\pi \mathrm{i} kx} = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi}\; e^{\mathrm{i} kx}$

- invertible **functions of** x as arguments: $\quad \delta\left[g(x) - g(a)\right] = \frac{\delta(x-a)}{|g'(a)|}$

  Proof: both sides have same effect in integrals

$$\int_{-\infty}^{\infty} \mathrm{d}x\; f(x) \left\{ \delta\left[g(x) - g(a)\right] - \frac{\delta(x-a)}{|g'(a)|} \right\} = \int_{-\infty}^{\infty} \mathrm{d}x\; g'(x) \frac{f(x)}{g'(x)} \delta\left[g(x) - g(a)\right] - \frac{f(a)}{|g'(a)|}$$

$$= \int_{g(-\infty)}^{g(\infty)} \mathrm{d}k\; \frac{f(g^{\mathrm{inv}}(k))}{g'(g^{\mathrm{inv}}(k))} \delta\left[k - g(a)\right] - \frac{f(a)}{|g'(a)|}$$

$$= sgn[g'(a)] \int_{-\infty}^{\infty} \mathrm{d}k\; \frac{f(g^{\mathrm{inv}}(k))}{g'(g^{\mathrm{inv}}(k))} \delta\left[k - g(a)\right] - \frac{f(a)}{|g'(a)|}$$

$$= sgn[g'(a)] \frac{f(a)}{g'(a)} - \frac{f(a)}{|g'(a)|} = 0$$

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Gaussian integrals

- one-dimensional:

$$\int \frac{\mathrm{d}x}{\sigma\sqrt{2\pi}}\, e^{-\frac{1}{2}x^2/\sigma^2} = 1, \qquad \int \frac{\mathrm{d}x}{\sigma\sqrt{2\pi}}\, x\, e^{-\frac{1}{2}x^2/\sigma^2} = 0, \qquad \int \frac{\mathrm{d}x}{\sigma\sqrt{2\pi}}\, x^2 e^{-\frac{1}{2}x^2/\sigma^2} = \sigma^2$$

$$\int \frac{\mathrm{d}x}{\sqrt{2\pi}}\, e^{kx-\frac{1}{2}x^2} = e^{\frac{1}{2}k^2} \quad (k \in \mathbb{C})$$

- N-dimensional:

$$\int \frac{\mathrm{d}\mathbf{x}}{\sqrt{(2\pi)^N \mathrm{det}\mathbf{C}}}\, e^{-\frac{1}{2}\mathbf{x}\cdot\mathbf{C}^{-1}\mathbf{x}} = 1, \qquad \int \frac{\mathrm{d}\mathbf{x}}{\sqrt{(2\pi)^N \mathrm{det}\mathbf{C}}}\, x_i e^{-\frac{1}{2}\mathbf{x}\cdot\mathbf{C}^{-1}\mathbf{x}} = 0,$$

$$\int \frac{\mathrm{d}\mathbf{x}}{\sqrt{(2\pi)^N \mathrm{det}\mathbf{C}}}\, x_i x_j e^{-\frac{1}{2}\mathbf{x}\cdot\mathbf{C}^{-1}\mathbf{x}} = C_{ij}$$

- multivariate Gaussian distribution:

$$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^N \mathrm{det}\mathbf{C}}}\, e^{-\frac{1}{2}\mathbf{x}\cdot\mathbf{C}^{-1}\mathbf{x}}$$

$$\int \mathrm{d}\mathbf{x}\; p(\mathbf{x}) x_i x_j = C_{ij}, \qquad \int \mathrm{d}\mathbf{x}\; p(\mathbf{x}) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = e^{-\frac{1}{2}\mathbf{k}\cdot\mathbf{C}\mathbf{k}}$$

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Steepest descent integration

Objective of steepest descent
(or 'saddle-point') integration:
large N behavior of integrals of the type

$$I_N = \int_{\mathbb{R}^p} \mathrm{d}\mathbf{x}\; g(\mathbf{x})\; e^{-Nf(\mathbf{x})}$$

- $f(\mathbf{x})$ real-valued, smooth, bounded from below,
  and with unique minimum at $\mathbf{x}^\star$

  expand f around minimum:

$$f(\mathbf{x}) = f(\mathbf{x}^\star) + \frac{1}{2}\sum_{ij=1}^{p} A_{ij}(x_i - x_i^\star)(x_j - x_j^\star) + \mathcal{O}(|\mathbf{x}-\mathbf{x}^\star|^3) \qquad A_{ij} = \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right|_{\mathbf{x}^\star}$$

  Insert into integral,
  transform $\mathbf{x} = \mathbf{x}^\star + \mathbf{y}/\sqrt{N}$:

$$\begin{aligned} I_N &= e^{-Nf(\mathbf{x}^\star)} \int_{\mathbb{R}^p} \mathrm{d}\mathbf{x}\; g(\mathbf{x}) e^{-\frac{1}{2}N\sum_{ij}(x_i - x_i^\star)A_{ij}(x_j - x_j^\star) + \mathcal{O}(N|\mathbf{x}-\mathbf{x}^\star|^3)} \\ &= N^{-\frac{p}{2}} e^{-Nf(\mathbf{x}^\star)} \int_{\mathbb{R}^p} \mathrm{d}\mathbf{y}\; g\Big(\mathbf{x}^\star + \frac{\mathbf{y}}{\sqrt{N}}\Big)\; e^{-\frac{1}{2}\sum_{ij} y_i A_{ij} y_j + \mathcal{O}(|\mathbf{y}|^3/\sqrt{N})} \end{aligned}$$

$$\int_{\mathbb{R}^p} \mathrm{d}\mathbf{x}\; g(\mathbf{x})\; e^{-Nf(\mathbf{x})} = N^{-\frac{p}{2}} e^{-Nf(\mathbf{x}^\star)} \int_{\mathbb{R}^p} \mathrm{d}\mathbf{y}\; g\Big(\mathbf{x}^\star + \frac{\mathbf{y}}{\sqrt{N}}\Big)\; e^{-\frac{1}{2}\sum_{ij} y_i A_{ij} y_j + \mathcal{O}(|\mathbf{y}|^3/\sqrt{N})}$$

- first result, for $p \ll N/\log N$:

$$-\lim_{N\to\infty} \frac{1}{N} \log \int_{\mathbb{R}^p} \mathrm{d}\mathbf{x}\; e^{-Nf(\mathbf{x})}$$

$$= f(\mathbf{x}^\star) + \lim_{N\to\infty} \Big[\frac{p \log N}{2N} - \frac{1}{N} \log \int_{\mathbb{R}^p} \mathrm{d}\mathbf{y}\; e^{-\frac{1}{2}\sum_{ij} y_i A_{ij} y_j + \mathcal{O}(|\mathbf{y}|^3/\sqrt{N})} \Big]$$

$$= f(\mathbf{x}^\star) + \lim_{N\to\infty} \Big[\frac{p \log N}{2N} - \frac{1}{2N} \log \Big(\frac{(2\pi)^p}{\det \mathbf{A}} \Big) - \frac{1}{N} \log \Big(1 + \mathcal{O}\big(\frac{p^{3/2}}{\sqrt{N}}\big) \Big) \Big]$$

$$= f(\mathbf{x}^\star) + \lim_{N\to\infty} \Big[\frac{p \log N}{2N} + \mathcal{O}\big(\frac{p}{N}\big) + \mathcal{O}\big(\frac{p^{3/2}}{N^{3/2}}\big) \Big] = f(\mathbf{x}^\star)$$

- second result, for $p \ll \sqrt{N}$:

$$\lim_{N\to\infty} \frac{\int \mathrm{d}\mathbf{x}\; g(\mathbf{x}) e^{-Nf(\mathbf{x})}}{\int \mathrm{d}\mathbf{x}\; e^{-Nf(\mathbf{x})}} = \lim_{N\to\infty} \Big[\frac{\int_{\mathbb{R}^p} \mathrm{d}\mathbf{y}\; g(\mathbf{x}^\star + \mathbf{y}/\sqrt{N})\; e^{-\frac{1}{2}\sum_{ij} y_i A_{ij} y_j + \mathcal{O}(|\mathbf{y}|^3/\sqrt{N})}}{\int_{\mathbb{R}^p} \mathrm{d}\mathbf{y}\; e^{-\frac{1}{2}\sum_{ij} y_i A_{ij} y_j + \mathcal{O}(|\mathbf{y}|^3/\sqrt{N})}} \Big]$$

$$= \frac{g(\mathbf{x}^\star)\Big(1 + \mathcal{O}\big(\frac{p}{\sqrt{N}}\big)\Big) \sqrt{\frac{(2\pi)^p}{\det \mathbf{A}}} \Big(1 + \mathcal{O}\big(\frac{p^{3/2}}{\sqrt{N}}\big)\Big)}{\sqrt{\frac{(2\pi)^p}{\det \mathbf{A}}} \Big(1 + \mathcal{O}\big(\frac{p^{3/2}}{\sqrt{N}}\big)\Big)} = g(\mathbf{x}^\star)$$

- $f(\mathbf{x})$ complex-valued:

  – deform integration path in complex plane, using Cauchy's theorem, such that along deformed path the imaginary part of $f(\mathbf{x})$ is constant, and preferably zero

  – proceed using Laplace's argument, and find the leading order in N by extremization of the real part of $f(\mathbf{x})$

  similar fomulae,
  but with (possibly complex) extrema
  that need no longer be maxima:

$$-\lim_{N\to\infty}\frac{1}{N}\log\int_{\mathbb{R}^p}\mathrm{d}\mathbf{x}\; e^{-Nf(\mathbf{x})} \;=\; \mathrm{extr}_{\mathbf{x}\in\mathbb{R}^p} f(\mathbf{x})$$

$$\lim_{N\to\infty}\frac{\int_{\mathbb{R}^p}\mathrm{d}\mathbf{x}\; g(\mathbf{x})e^{-Nf(\mathbf{x})}}{\int_{\mathbb{R}^p}\mathrm{d}\mathbf{x}\; e^{-Nf(\mathbf{x})}} = g\Big(\arg\,\mathrm{extr}_{\mathbf{x}\in\mathbb{R}^p} f(\mathbf{x})\Big)$$

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Exponential distributions

Often we study stochastic processes for $\mathbf{x} \in X \subseteq \mathbb{R}^N$,
that evolve to a stationary state, with prob distribution $p(\mathbf{x})$
many are of the following form:

- stationary state is *minimally informative*,
  subject to a number of constraints

$$\sum_{\mathbf{x}\in X} p(\mathbf{x})\omega_1(\mathbf{x}) = \Omega_1 \quad \ldots\ldots \quad \sum_{\mathbf{x}\in X} p(\mathbf{x})\omega_L(\mathbf{x}) = \Omega_L$$

This is enough to calculate $p(\mathbf{x})$:

- information content of $\mathbf{x}$: Shannon entropy
  hence

$$\textit{maximize} \quad S = -\sum_{\mathbf{x}\in X} p(\mathbf{x}) \log p(\mathbf{x})$$

$$\textit{subject to}: \quad \left\{ \begin{array}{l} p(\mathbf{x}) \geq 0 \ \ \forall \mathbf{x}, \ \ \sum_{\mathbf{x}\in X} p(\mathbf{x}) = 1 \\ \sum_{\mathbf{x}\in X} p(\mathbf{x})\omega_\ell(\mathbf{x}) = \Omega_\ell \ \ \textit{for all } \ell = 1 \ldots L \end{array} \right.$$

- solution using Lagrange's method:

$$\frac{\partial}{\partial p(\mathbf{x})}\Big\{\lambda_0\sum_{\mathbf{x}'\in X}p(\mathbf{x}')+\sum_{\ell=1}^{L}\lambda_\ell\sum_{\mathbf{x}'\in X}p(\mathbf{x}')\omega_\ell(\mathbf{x}')-\sum_{\mathbf{x}'\in X}p(\mathbf{x}')\log p(\mathbf{x}')\Big\}=0$$

$$\lambda_0+\sum_{\ell=1}^{L}\lambda_\ell\omega_\ell(\mathbf{x})-1-\log p(\mathbf{x})=0 \quad\Rightarrow\quad p(\mathbf{x})=\mathrm{e}^{\lambda_0-1+\sum_{\ell=1}^{L}\lambda_\ell\omega_\ell(\mathbf{x})}$$

$$(p(\mathbf{x})\geq 0\ \ \textit{automatically satisfied})$$

- 'exponential distribution':

$$p(\mathbf{x})=\frac{\mathrm{e}^{\sum_{\ell=1}^{L}\lambda_\ell\omega_\ell(\mathbf{x})}}{Z(\boldsymbol{\lambda})},\qquad Z(\boldsymbol{\lambda})=\sum_{\mathbf{x}\in X}\mathrm{e}^{\sum_{\ell=1}^{L}\lambda_\ell\omega_\ell(\mathbf{x})}$$

$$\boldsymbol{\lambda}=(\lambda_1,\ldots,\lambda_L):\quad \textit{solved from}\quad \sum_{\mathbf{x}\in X}p(\mathbf{x})\omega_\ell(\mathbf{x})=\Omega_\ell\quad(\ell=1\ldots L)$$

example:
physical systems in thermal equilibrium
$L=1$, $\omega(\mathbf{x})=E(\mathbf{x})$ (energy), $\lambda=-1/k_BT$

$$p(\mathbf{x})=\frac{\mathrm{e}^{-E(\mathbf{x})/k_BT}}{Z(T)},\qquad Z(T)=\sum_{\mathbf{x}\in X}\mathrm{e}^{-E(\mathbf{x})/k_BT}$$

Generating functions

$$p(\mathbf{x}) = \frac{e^{\sum_{\ell=1}^{L} \lambda_\ell \omega_\ell(\mathbf{x})}}{Z(\boldsymbol{\lambda})}, \qquad Z(\boldsymbol{\lambda}) = \sum_{\mathbf{x}\in X} e^{\sum_{\ell=1}^{L} \lambda_\ell \omega_\ell(\mathbf{x})}, \qquad \langle f\rangle = \sum_{\mathbf{x}\in X} p(\mathbf{x}) f(\mathbf{x})$$

Idea behind generating functions:
reduce nr of state averages to be calculated ...

- define
  $F(\boldsymbol{\lambda}) = \log Z(\boldsymbol{\lambda})$
  $$\frac{\partial F(\boldsymbol{\lambda})}{\partial \lambda_k} = \frac{\sum_{\mathbf{x}\in X} \omega_k(\mathbf{x}) e^{\sum_{\ell=1}^{L} \lambda_\ell \omega_\ell(\mathbf{x})}}{\sum_{\mathbf{x}\in X} e^{\sum_{\ell=1}^{L} \lambda_\ell \omega_\ell(\mathbf{x})}} = \langle \omega_k(\mathbf{x})\rangle$$

- how to calculate
  arbitrary state average $\langle\psi\rangle$?

$$F(\boldsymbol{\lambda}, \mu) = \log\Big[\sum_{\mathbf{x}\in X} e^{\mu\psi(\mathbf{x}) + \sum_\ell \lambda_\ell \omega_\ell(\mathbf{x})}\Big]$$

$$\langle\psi\rangle = \lim_{\mu\to 0} \frac{\partial F(\boldsymbol{\lambda}, \mu)}{\partial \mu}, \qquad \langle \omega_\ell\rangle = \lim_{\mu\to 0} \frac{\partial F(\boldsymbol{\lambda}, \mu)}{\partial \lambda_\ell}$$

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The replica trick

first appearance: Marc Kac 1968
first application in physics: Sherrington & Kirkpatrick 1975
first application in biology: Amit, Gutfreund & Sompolinksy 1985

- Consider processes with many fixed (pseudo-)random parameters $\boldsymbol{\xi}$, distributed according to $\mathcal{P}(\boldsymbol{\xi})$

$$p(\mathbf{x}|\boldsymbol{\xi}) = \frac{\mathrm{e}^{\sum_{\ell=1}^{L} \lambda_\ell \omega_\ell(\mathbf{x},\boldsymbol{\xi})}}{Z(\boldsymbol{\lambda},\boldsymbol{\xi})}, \qquad Z(\boldsymbol{\lambda},\boldsymbol{\xi}) = \sum_{\mathbf{x}\in X} \mathrm{e}^{\sum_{\ell=1}^{L} \lambda_\ell \omega_\ell(\mathbf{x},\boldsymbol{\xi})}$$

  – calculating state averages $\langle f\rangle_{\boldsymbol{\xi}}$ for each realisation of $\boldsymbol{\xi}$ is usually impossible

  – we are mostly interested in *typical* values of state averages

  – for $N\to\infty$ macroscopic averages will not depend on $\boldsymbol{\xi}$, only on $\mathcal{P}(\boldsymbol{\xi})$, 'self-averaging': $\lim_{N\to\infty}\langle f\rangle_{\boldsymbol{\xi}}$ indep of $\boldsymbol{\xi}$

so focus on

$$\overline{\langle f\rangle_{\boldsymbol{\xi}}} = \sum_{\boldsymbol{\xi}} \mathcal{P}(\boldsymbol{\xi})\langle f\rangle_{\boldsymbol{\xi}} = \sum_{\boldsymbol{\xi}} \mathcal{P}(\boldsymbol{\xi})\Big\{\sum_{\mathbf{x}\in X} p(\mathbf{x}|\boldsymbol{\xi}) f(\mathbf{x},\boldsymbol{\xi})\Big\}$$

- new generating function:

$$\overline{F}(\boldsymbol{\lambda},\mu)=\sum_{\boldsymbol{\xi}}\mathcal{P}(\boldsymbol{\xi})\log Z(\boldsymbol{\lambda},\mu,\boldsymbol{\xi}),\qquad Z(\boldsymbol{\lambda},\mu,\boldsymbol{\xi})=\sum_{\mathbf{x}\in X}\mathrm{e}^{\mu\psi(\mathbf{x},\boldsymbol{\xi})+\sum_\ell\lambda_\ell\omega_\ell(\mathbf{x},\boldsymbol{\xi})}$$

$$\lim_{\mu\to0}\frac{\partial}{\partial\mu}\overline{F}(\boldsymbol{\lambda},\mu)=\lim_{\mu\to0}\sum_{\boldsymbol{\xi}}\mathcal{P}(\boldsymbol{\xi})\left\{\frac{\sum_{\mathbf{x}\in X}\psi(\mathbf{x},\boldsymbol{\xi})\mathrm{e}^{\mu\psi(\mathbf{x},\boldsymbol{\xi})+\sum_\ell\lambda_\ell\omega_\ell(\mathbf{x},\boldsymbol{\xi})}}{\sum_{\mathbf{x}\in X}\mathrm{e}^{\mu\psi(\mathbf{x},\boldsymbol{\xi})+\sum_\ell\lambda_\ell\omega_\ell(\mathbf{x},\boldsymbol{\xi})}}\right\}$$

$$=\sum_{\boldsymbol{\xi}}\mathcal{P}(\boldsymbol{\xi})\left\{\frac{\sum_{\mathbf{x}\in X}\psi(\mathbf{x},\boldsymbol{\xi})\mathrm{e}^{\sum_\ell\lambda_\ell\omega_\ell(\mathbf{x},\boldsymbol{\xi})}}{\sum_{\mathbf{x}\in X}\mathrm{e}^{\sum_\ell\lambda_\ell\omega_\ell(\mathbf{x},\boldsymbol{\xi})}}\right\}=\overline{\langle\psi\rangle_{\boldsymbol{\xi}}}$$

- main obstacle in calculating $\overline{F}$:
  the logarithm ...

  replica identity : $\overline{\log Z}=\lim_{n\to0}\frac{1}{n}\log\overline{Z^n}$

  proof:

$$\begin{aligned}\lim_{n\to0}\frac{1}{n}\log\overline{Z^n}&=\lim_{n\to0}\frac{1}{n}\log\overline{[\mathrm{e}^{n\log Z}]}=\lim_{n\to0}\frac{1}{n}\log\overline{[1+n\log Z+\mathcal{O}(n^2)]}\\&=\lim_{n\to0}\frac{1}{n}\log[1+n\overline{\log Z}+\mathcal{O}(n^2)]=\overline{\log Z}\end{aligned}$$

- apply $\overline{\log Z} = \lim_{n\to 0} \frac{1}{n} \log \overline{Z^n}$
  (simplest case $L = 1$)

$$
\begin{aligned}
\overline{F}(\lambda) &= \sum_{\boldsymbol{\xi}} \mathcal{P}(\boldsymbol{\xi}) \log\Big[\sum_{\mathbf{x}\in X} e^{\lambda\omega(\mathbf{x},\boldsymbol{\xi})}\Big] = \lim_{n\to 0} \frac{1}{n} \log \sum_{\boldsymbol{\xi}} \mathcal{P}(\boldsymbol{\xi}) \Big[\sum_{\mathbf{x}\in X} e^{\lambda\omega(\mathbf{x},\boldsymbol{\xi})}\Big]^n \\
&= \lim_{n\to 0} \frac{1}{n} \log \sum_{\boldsymbol{\xi}} \mathcal{P}(\boldsymbol{\xi}) \Big[\sum_{\mathbf{x}^1\in X} \cdots \sum_{\mathbf{x}^n\in X} e^{\lambda \sum_{\alpha=1}^n \omega(\mathbf{x}^\alpha,\boldsymbol{\xi})}\Big] \\
&= \lim_{n\to 0} \frac{1}{n} \log \Big[\sum_{\mathbf{x}^1\in X} \cdots \sum_{\mathbf{x}^n\in X} \sum_{\boldsymbol{\xi}} \mathcal{P}(\boldsymbol{\xi}) e^{\lambda \sum_{\alpha=1}^n \omega(\mathbf{x}^\alpha,\boldsymbol{\xi})}\Big]
\end{aligned}
$$

- notes:
  - impossible $\boldsymbol{\xi}$-average converted into simpler one ...
  - calculation involves n 'replicas' $\mathbf{x}^\alpha$ of original system
  - but $n \to 0$ at the end ... ?
  - penultimate step true only for *integer n*,
    so limit requires *analytical continuation* ...

since then: alternative (more tedious) routes,
these confirmed correctness of the replica method!

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The replica trick and algorithms

Suppose we have data D, with prob distr $\mathcal{P}(D)$
and an algorithm which minimises an error function $E(D,\boldsymbol{\theta})$
(maximum likelihood, Cox & Bayesian regression, SVM, perceptron, ...)

- algorithm outcome:

$$\boldsymbol{\theta}^{\star}(D)=\arg\min_{\boldsymbol{\theta}}E(D,\boldsymbol{\theta}),\qquad E_{\rm min}(D)=\min_{\boldsymbol{\theta}}E(D,\boldsymbol{\theta})$$

  typical performance:

$$\boldsymbol{\theta}^{\star}=\sum_{D}\mathcal{P}(D)\boldsymbol{\theta}^{\star}(D)=\overline{\boldsymbol{\theta}^{\star}(D)}\qquad E_{\rm min}=\sum_{D}\mathcal{P}(D)E_{\rm min}(D)=\overline{E_{\rm min}(D)}$$

- steepest descent identity & replica trick:

$$\begin{aligned}
E_{\rm min}(D) &= \min_{\boldsymbol{\theta}}E(D,\boldsymbol{\theta})=-\lim_{\beta\to\infty}\frac{1}{\beta}\log\int\!{\rm d}\boldsymbol{\theta}\;{\rm e}^{-\beta E(D,\boldsymbol{\theta})}\\
E_{\rm min} &= \overline{E_{\rm min}(D)}=-\lim_{\beta\to\infty}\frac{1}{\beta}\overline{\log\int\!{\rm d}\boldsymbol{\theta}\;{\rm e}^{-\beta E(D,\boldsymbol{\theta})}}\\
&= -\lim_{\beta\to\infty}\lim_{n\to 0}\frac{1}{\beta n}\log\overline{\Big[\int\!{\rm d}\boldsymbol{\theta}\;{\rm e}^{-\beta E(D,\boldsymbol{\theta})}\Big]^{n}}\\
&= -\lim_{\beta\to\infty}\lim_{n\to 0}\frac{1}{\beta n}\log\int\!{\rm d}\boldsymbol{\theta}^{1}\ldots\boldsymbol{\theta}^{n}\;\overline{{\rm e}^{-\beta\sum_{\alpha=1}^{n}E(D,\boldsymbol{\theta}^{\alpha})}}
\end{aligned}$$

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Alternative forms of the replica identity

suppose we need averages, but for
a $p(\mathbf{x}|\boldsymbol{\xi})$ that is not of an exponential form?

or we need to average quantities that we
don't want in the exponent of $Z(\lambda\boldsymbol{\xi})$?

$$p(\mathbf{x}|\boldsymbol{\xi}) = \frac{W(\mathbf{x},\boldsymbol{\xi})}{\sum_{\mathbf{x}'\in X} W(\mathbf{x}',\boldsymbol{\xi})}, \qquad \overline{\langle f\rangle_{\boldsymbol{\xi}}} = \overline{\sum_{\mathbf{x}\in X} p(\mathbf{x}|\boldsymbol{\xi}) f(\mathbf{x},\boldsymbol{\xi})}$$

- main obstacle here:
  the fraction ...

$$\begin{aligned}
\overline{\langle f\rangle_{\boldsymbol{\xi}}} &= \overline{\left[\frac{\sum_{\mathbf{x}\in X} W(\mathbf{x},\boldsymbol{\xi}) f(\mathbf{x},\boldsymbol{\xi})}{\sum_{\mathbf{x}\in X} W(\mathbf{x},\boldsymbol{\xi})}\right]} = \overline{\Big[\sum_{\mathbf{x}\in X} W(\mathbf{x},\boldsymbol{\xi}) f(\mathbf{x},\boldsymbol{\xi})\Big]\Big[\sum_{\mathbf{x}\in X} W(\mathbf{x},\boldsymbol{\xi})\Big]^{-1}} \\
&= \lim_{n\to 0} \overline{\Big[\sum_{\mathbf{x}\in X} W(\mathbf{x},\boldsymbol{\xi}) f(\mathbf{x},\boldsymbol{\xi})\Big]\Big[\sum_{\mathbf{x}\in X} W(\mathbf{x},\boldsymbol{\xi})\Big]^{n-1}} \\
&= \lim_{n\to 0} \sum_{\mathbf{x}^1\in X} \cdots \sum_{\mathbf{x}^n\in X} \overline{f(\mathbf{x}^1,\boldsymbol{\xi}) W(\mathbf{x}^1,\boldsymbol{\xi}) \ldots W(\mathbf{x}^n,\boldsymbol{\xi})}
\end{aligned}$$

(again: used integer n, but $n \to 0$ ...)

- equivalence between two forms of replica identity, if $$W(\mathbf{x},\boldsymbol{\xi}) = \mathrm{e}^{\sum_\ell \lambda_\ell \phi_\ell(\mathbf{x},\boldsymbol{\xi})}$$

proof:

$$
\begin{aligned}
\overline{\langle f\rangle_{\boldsymbol{\xi}}} &= \lim_{n\to 0} \sum_{\mathbf{x}^1\in X}\cdots\sum_{\mathbf{x}^n\in X} \overline{f(\mathbf{x}^1,\boldsymbol{\xi})W(\mathbf{x}^1,\boldsymbol{\xi})\ldots W(\mathbf{x}^n,\boldsymbol{\xi})} \\
&= \lim_{n\to 0} \sum_{\mathbf{x}^1\in X}\cdots\sum_{\mathbf{x}^n\in X} \overline{f(\mathbf{x}^1,\boldsymbol{\xi})\,\mathrm{e}^{\sum_{\alpha=1}^n \sum_\ell \lambda_\ell\phi_\ell(\mathbf{x}^\alpha,\boldsymbol{\xi})}} \\
&= \lim_{n\to 0} \frac{1}{n} \sum_{\mathbf{x}^1\in X}\cdots\sum_{\mathbf{x}^n\in X} \overline{\Big[\sum_{\alpha=1}^n f(\mathbf{x}^\alpha,\boldsymbol{\xi})\Big]\,\mathrm{e}^{\sum_{\alpha=1}^n \sum_\ell \lambda_\ell\phi_\ell(\mathbf{x}^\alpha,\boldsymbol{\xi})}} \\
&= \lim_{n\to 0} \frac{1}{n} \lim_{\mu\to 0} \frac{\partial}{\partial\mu} \sum_{\mathbf{x}^1\in X}\cdots\sum_{\mathbf{x}^n\in X} \overline{\mathrm{e}^{\sum_{\alpha=1}^n \sum_\ell \lambda_\ell\phi_\ell(\mathbf{x}^\alpha,\boldsymbol{\xi})+\mu\sum_{\alpha=1}^n f(\mathbf{x}^\alpha,\boldsymbol{\xi})}} \\
&= \lim_{\mu\to 0} \frac{\partial}{\partial\mu} \lim_{n\to 0} \frac{1}{n} \overline{\sum_{\mathbf{x}^1\in X}\cdots\sum_{\mathbf{x}^n\in X} \mathrm{e}^{\sum_{\alpha=1}^n \left[\sum_\ell \lambda_\ell\phi_\ell(\mathbf{x}^\alpha,\boldsymbol{\xi})+\mu f(\mathbf{x}^\alpha,\boldsymbol{\xi})\right]}} \\
&= \lim_{\mu\to 0} \frac{\partial}{\partial\mu} \lim_{n\to 0} \frac{1}{n}\overline{Z^n(\boldsymbol{\lambda},\mu,\boldsymbol{\xi})}, \qquad Z(\boldsymbol{\lambda},\mu,\boldsymbol{\xi}) = \sum_{\mathbf{x}\in X} \mathrm{e}^{\sum_\ell \lambda_\ell\phi_\ell(\mathbf{x},\boldsymbol{\xi})+\mu f(\mathbf{x},\boldsymbol{\xi})}
\end{aligned}
$$

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Attractor neural networks

$N \sim 10^{12-14}$ brain cells (neurons),
each connected with $\sim 10^{3-5}$ others

- **neurons**

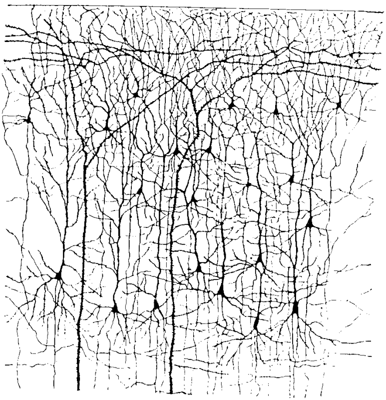
  two states:
  $\sigma_i = 1$ (i fires electric pulses)
  $\sigma_i = -1$ (i is at rest)

- **dynamics of firing states**

$$\sigma_i(t+1) = sgn\Big[\overbrace{\sum_{j=1}^{N} J_{ij}\sigma_j(t)}^{activation\ signal} + \overbrace{\theta_i + z_i(t)}^{threshold,\ noise} \Big]$$

$\theta_i \in \mathbb{R}$: *firing threshold of neuron i*
$J_{ij} \in \mathbb{R}$: *synaptic connection* $j \to i$

learning = adaptation of $\{J_{ij}, \theta_i\}$



non-local 'distributed' storage of 'program' and 'data'

attractor neural networks

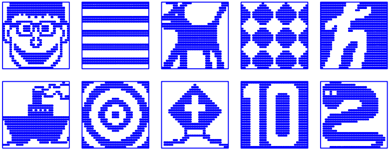
models for associative memory in the brain

- **the neural code**

  represent ‘patterns’ as
  micro-states $\boldsymbol{\xi}=(\xi_1,\ldots,\xi_N)$

  $\circ$: $\sigma_i=-1$, $\bullet$: $\sigma_i=1$

  e.g. $N=400$,
  10 patterns:



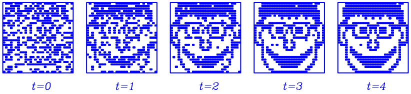
- **information storage**

  modify synapses $\{J_{ij}\}$ such that $\boldsymbol{\xi}$ is
  stable state (attractor) of the neuronal dynamics

- **information recall**

  initial state $\boldsymbol{\sigma}(t=0)$:
  evolution to nearest attractor

  if $\boldsymbol{\sigma}(0)$ close (i.e. similar) to $\boldsymbol{\xi}$:
  $\boldsymbol{\sigma}(t=\infty)=\boldsymbol{\xi}$



- learning rule: recipe for storing patterns via modification of $\{J_{ij}\}$
Hebb (1949): $\Delta J_{ij} \propto \xi_i \xi_j$

choose $J_{ij} = J_0 \xi_i \xi_j$, $\theta_i = 0$,
update randomly drawn i at each step:

$$\sigma_i(t+1) = sgn\Big[\sum_{j=1}^{N} J_{ij}\sigma_j(t) + z_i(t)\Big] = sgn\Big[J_0\xi_i \overbrace{\Big(\sum_{j=1}^{N}\xi_j\sigma_j(t)\Big)}^{\text{pattern overlap}} + z_i(t)\Big]$$

$$= \xi_i \; sgn\Big[J_0 \sum_{j=1}^{N}\xi_j\sigma_j(t) + \xi_i z_i(t)\Big]$$

$M(t) = \sum_{j=1}^{N} \xi_j\sigma_j(t)$ sufficiently large: $\sigma_i(t+1) = \xi_i$
now $M(t+1) \geq M(t)$ ...
will continue until $\boldsymbol{\sigma} = \boldsymbol{\xi}$

- proper analysis:

noise: $P(z) = \frac{\beta}{2}[1 - \tanh^2(\beta z)]$,
symmetric synapses: $J_{ij} = J_{ji}$, $J_{ii} = 0$
sequential updates of σ_i

$$p(\boldsymbol{\sigma}) = \frac{e^{-\beta H(\boldsymbol{\sigma})}}{Z(\beta)}, \qquad H(\boldsymbol{\sigma}) = -\frac{1}{2}\sum_{i \neq j} \sigma_i J_{ij}\sigma_j - \sum_i \theta_i\sigma_i$$

a more realistic model,
solvable via the replica method

- **storage of a pattern $\boldsymbol{\xi}=(\xi_1,\ldots,\xi_N)\in\{-1,1\}^N$**
  on background of zero-average Gaussian synapses

$$J_{ij}=\frac{J_0}{N}\xi_i\xi_j+\frac{J}{\sqrt{N}}z_{ij},\qquad \overline{z_{ij}}=0,\ \overline{z_{ij}^2}=1,\quad J,J_0\geq 0,\quad \theta_i=0$$

  to be averaged over: background synapses $\{z_{ij}\}$
  pattern overlap: $m(\boldsymbol{\sigma})=\frac{1}{N}\sum_k \sigma_k\xi_k$

$$\begin{aligned}
H(\boldsymbol{\sigma}) &= -\frac{1}{2}\sum_{i\neq j}\sigma_i\sigma_j\Big\{\frac{J_0}{N}\xi_i\xi_j+\frac{J}{\sqrt{N}}z_{ij}\Big\}\\
&= -\frac{J_0}{2N}\sum_{ij}\sigma_i\sigma_j\xi_i\xi_j+\frac{J_0}{2N}\sum_i 1-\frac{J}{2\sqrt{N}}\sum_{i\neq j}\sigma_i\sigma_j z_{ij}\\
&= -\frac{1}{2}NJ_0m^2(\boldsymbol{\sigma})+\frac{1}{2}J_0-\frac{J}{\sqrt{N}}\sum_{i<j}\sigma_i\sigma_j z_{ij}
\end{aligned}$$

- **generating function**

$$\overline{F}=\overline{\log Z(\beta)}=\lim_{n\to 0}\frac{1}{n}\log\overline{Z^n(\beta)}=\lim_{n\to 0}\frac{1}{n}\log\Big[\sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n}\overline{e^{-\beta\sum_{\alpha=1}^n H(\boldsymbol{\sigma}^\alpha)}}\Big]$$

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The replica calculation

short-hands: $m(\boldsymbol{\sigma}) = \frac{1}{N}\sum_i \xi_i \sigma_i, \quad \mathrm{D}z = (2\pi)^{-1/2} \mathrm{e}^{-z^2/2} \mathrm{d}z$

Gaussian integral: $\int \mathrm{D}z\, \mathrm{e}^{xz} = \mathrm{e}^{\frac{1}{2}x^2}$

- **average over random synapses**

$$
\begin{aligned}
\overline{Z^n(\beta)} &= \sum_{\boldsymbol{\sigma}^1 \ldots \boldsymbol{\sigma}^n} \overline{\mathrm{e}^{-\beta \sum_{\alpha=1}^n H(\boldsymbol{\sigma}^\alpha)}} \\
&= \sum_{\boldsymbol{\sigma}^1 \ldots \boldsymbol{\sigma}^n} \overline{\mathrm{e}^{-\beta \sum_{\alpha=1}^n \left[\frac{1}{2}J_0 - \frac{1}{2}NJ_0 m^2(\boldsymbol{\sigma}^\alpha) - \frac{J}{\sqrt{N}} \sum_{i<j} \sigma_i^\alpha \sigma_j^\alpha z_{ij}\right]}} \\
&= e^{-\frac{1}{2}n\beta J_0} \sum_{\boldsymbol{\sigma}^1 \ldots \boldsymbol{\sigma}^n} \mathrm{e}^{\frac{1}{2}N\beta J_0 \sum_{\alpha=1}^n m^2(\boldsymbol{\sigma}^\alpha)} \overline{\mathrm{e}^{\frac{\beta J}{\sqrt{N}} \sum_{\alpha=1}^n \sum_{i<j} \sigma_i^\alpha \sigma_j^\alpha z_{ij}}} \\
&= e^{-\frac{1}{2}n\beta J_0} \sum_{\boldsymbol{\sigma}^1 \ldots \boldsymbol{\sigma}^n} \mathrm{e}^{\frac{1}{2}N\beta J_0 \sum_{\alpha=1}^n m^2(\boldsymbol{\sigma}^\alpha)} \prod_{i<j} \int \mathrm{D}z\, \mathrm{e}^{\frac{\beta J}{\sqrt{N}} \sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha z} \\
&= e^{-\frac{1}{2}n\beta J_0} \sum_{\boldsymbol{\sigma}^1 \ldots \boldsymbol{\sigma}^n} \mathrm{e}^{\frac{1}{2}N\beta J_0 \sum_{\alpha=1}^n m^2(\boldsymbol{\sigma}^\alpha)} \prod_{i<j} \mathrm{e}^{\frac{\beta^2 J^2}{2N}\left[\sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha\right]^2} \\
&= e^{-\frac{1}{2}n\beta J_0} \sum_{\boldsymbol{\sigma}^1 \ldots \boldsymbol{\sigma}^n} \mathrm{e}^{N\left[\frac{1}{2}\beta J_0 \sum_{\alpha=1}^n m^2(\boldsymbol{\sigma}^\alpha) + \frac{1}{2}(\beta J)^2 \sum_{\alpha,\gamma=1}^n \left(N^{-2}\sum_{i<j} \sigma_i^\alpha \sigma_j^\alpha \sigma_i^\gamma \sigma_j^\gamma\right)\right]}
\end{aligned}
$$

- **complete square** in sums over neurons

$$\sum_{i<j}\sigma_i^\alpha\sigma_j^\alpha\sigma_i^\gamma\sigma_j^\gamma = \frac{1}{2}\sum_{i\neq j}\sigma_i^\alpha\sigma_j^\alpha\sigma_i^\gamma\sigma_j^\gamma = \frac{1}{2}\sum_{ij}\sigma_i^\alpha\sigma_j^\alpha\sigma_i^\gamma\sigma_j^\gamma - \frac{1}{2}\sum_i 1$$
$$= \frac{1}{2}\Big(\sum_i \sigma_i^\alpha\sigma_i^\gamma\Big)^2 - \frac{1}{2}N$$

hence

$$\overline{Z^n(\beta)} = e^{-\frac{1}{2}n\beta J_0}\sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n} \mathrm{e}^{N\left[\frac{1}{2}\beta J_0\sum_{\alpha=1}^n m^2(\boldsymbol{\sigma}^\alpha)+\frac{1}{4}(\beta J)^2\sum_{\alpha,\gamma=1}^n\left(\left(\frac{1}{N}\sum_i\sigma_i^\alpha\sigma_i^\gamma\right)^2-\frac{1}{N}\right)\right]}$$
$$= e^{-\frac{1}{2}n\beta J_0-\frac{1}{4}n(\beta J)^2}\sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n} \mathrm{e}^{N\left[\frac{1}{2}\beta J_0\sum_{\alpha=1}^n m^2(\boldsymbol{\sigma}^\alpha)+\frac{1}{4}(\beta J)^2\sum_{\alpha,\gamma=1}^n\left(\frac{1}{N}\sum_i\sigma_i^\alpha\sigma_i^\gamma\right)^2\right]}$$

- insert:

$$1=\prod_{\alpha=1}^n\int \mathrm{d}m_\alpha\;\delta\Big(m_\alpha-\frac{1}{N}\sum_i\xi_i\sigma_i^\alpha\Big),\qquad 1=\prod_{\alpha,\gamma=1}^n\int \mathrm{d}q_{\alpha\gamma}\;\delta\Big(q_{\alpha\gamma}-\frac{1}{N}\sum_i\sigma_i^\alpha\sigma_i^\gamma\Big)$$

$\mathbf{m}\in\mathbb{R}^n$, $\mathbf{q}\in\mathbb{R}^{n^2}$:

$$\overline{Z^n(\beta)} = e^{-\frac{1}{2}n\beta J_0-\frac{1}{4}n(\beta J)^2}\int \mathrm{d}\mathbf{m}\mathrm{d}\mathbf{q}\; e^{N\left[\frac{1}{2}\beta J_0\sum_{\alpha=1}^n m_\alpha^2+\frac{1}{4}(\beta J)^2\sum_{\alpha,\gamma=1}^n q_{\alpha\gamma}^2\right]}$$
$$\times\sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n}\Big[\prod_{\alpha=1}^n\delta\Big(m_\alpha-\frac{1}{N}\sum_i\xi_i\sigma_i^\alpha\Big)\Big]\Big[\prod_{\alpha,\gamma=1}^n\delta\Big(q_{\alpha\gamma}-\frac{1}{N}\sum_i\sigma_i^\alpha\sigma_i^\gamma\Big)\Big]$$

remember: $\delta(x) = (2\pi)^{-1} \int \mathrm{d}\hat{x}\ \mathrm{e}^{\mathrm{i}x\hat{x}}$

- the **sum over neuron state variables**

$$\sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n} \Big[\prod_{\alpha=1}^n \delta\Big(m_\alpha - \frac{1}{N}\sum_i \xi_i\sigma_i^\alpha\Big)\Big]\Big[\prod_{\alpha,\gamma=1}^n \delta\Big(q_{\alpha\gamma} - \frac{1}{N}\sum_i \sigma_i^\alpha\sigma_i^\gamma\Big)\Big]$$

$$= \sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n} \int \frac{\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}}{(2\pi)^{n^2+n}} \mathrm{e}^{\mathrm{i}\sum_{\alpha=1}^n \hat{m}_\alpha\left[m_\alpha - \frac{1}{N}\sum_i \xi_i\sigma_i^\alpha\right] + \mathrm{i}\sum_{\alpha,\gamma=1}^n \hat{q}_{\alpha\gamma}\left[q_{\alpha\gamma} - \frac{1}{N}\sum_i \sigma_i^\alpha\sigma_i^\gamma\right]}$$

$$= \int \frac{\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}}{(2\pi)^{n(n+1)}}\ \mathrm{e}^{\mathrm{i}\sum_\alpha \hat{m}_\alpha m_\alpha + \mathrm{i}\sum_{\alpha\gamma}\hat{q}_{\alpha\gamma}q_{\alpha\gamma}} \sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n}\prod_{i=1}^N \mathrm{e}^{-\frac{\mathrm{i}}{N}\left[\sum_\alpha \hat{m}_\alpha\xi_i\sigma_i^\alpha + \sum_{\alpha\gamma}\hat{q}_{\alpha\gamma}\sigma_i^\alpha\sigma_i^\gamma\right]}$$

$$= \int \frac{\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}}{(2\pi)^{n(n+1)}}\ \mathrm{e}^{\mathrm{i}\sum_\alpha \hat{m}_\alpha m_\alpha + \mathrm{i}\sum_{\alpha\gamma}\hat{q}_{\alpha\gamma}q_{\alpha\gamma}} \prod_i \sum_{\sigma_1\ldots\sigma_n} \mathrm{e}^{-\frac{\mathrm{i}}{N}\left[\sum_\alpha \hat{m}_\alpha\xi_i\sigma_\alpha + \sum_{\alpha\gamma}\hat{q}_{\alpha\gamma}\sigma_\alpha\sigma_\gamma\right]}$$

transform: $\hat{\mathbf{m}} \to N\hat{\mathbf{m}}$, $\hat{\mathbf{q}} \to N\hat{\mathbf{q}}$, $\sigma_\alpha \to \xi_i\sigma_\alpha$:

$$\sum_{\boldsymbol{\sigma}^1\ldots\boldsymbol{\sigma}^n}\Big[\ldots\Big]\Big[\ldots\Big] = \int \frac{\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}}{(2\pi/N)^{n(n+1)}}\ \mathrm{e}^{\mathrm{i}N\left[\hat{\mathbf{m}}\cdot\mathbf{m} + \mathrm{Tr}(\hat{\mathbf{q}}\mathbf{q})\right]}\Big[\sum_{\boldsymbol{\sigma}\in\{-1,1\}^n} \mathrm{e}^{-\mathrm{i}\hat{\mathbf{m}}\cdot\boldsymbol{\sigma} - \mathrm{i}\boldsymbol{\sigma}\cdot\hat{\mathbf{q}}\boldsymbol{\sigma}}\Big]^N$$

$$= \int \frac{\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}}{(2\pi/N)^{n(n+1)}}\ \mathrm{e}^{\mathrm{i}N\hat{\mathbf{m}}\cdot\mathbf{m} + \mathrm{i}N\mathrm{Tr}(\hat{\mathbf{q}}\mathbf{q}) + N\log\sum_{\boldsymbol{\sigma}}\exp(-\mathrm{i}\hat{\mathbf{m}}\cdot\boldsymbol{\sigma} - \mathrm{i}\boldsymbol{\sigma}\cdot\hat{\mathbf{q}}\boldsymbol{\sigma})}$$

- combine everything ...

$$\overline{Z^n(\beta)} = e^{-\frac{1}{2}n\beta J_0 - \frac{1}{4}n(\beta J)^2 - n(n+1)\log(2\pi/N)} \int \mathrm{d}\mathbf{m}\mathrm{d}\mathbf{q}\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}\ \mathrm{e}^{N\Psi(\mathbf{m},\mathbf{q},\hat{\mathbf{m}},\hat{\mathbf{q}})}$$

$$\Psi(\ldots) = \frac{1}{2}\beta J_0 \mathbf{m}^2 + \frac{1}{4}(\beta J)^2 \mathrm{Tr}(\mathbf{q}^2) + \mathrm{i}\hat{\mathbf{m}}\cdot\mathbf{m} + \mathrm{i}\mathrm{Tr}(\hat{\mathbf{q}}\mathbf{q}) + \log\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\mathrm{i}\hat{\mathbf{m}}\cdot\boldsymbol{\sigma} - \mathrm{i}\boldsymbol{\sigma}\cdot\hat{\mathbf{q}}\boldsymbol{\sigma}}$$

Hence

$$\begin{aligned}\overline{F} &= \lim_{n\to 0}\frac{1}{n}\log\overline{Z^n(\beta)} \\ &= -\frac{1}{2}\beta J_0 - \frac{1}{4}(\beta J)^2 - \log(\frac{2\pi}{N}) + \lim_{n\to 0}\frac{1}{n}\log\int \mathrm{d}\mathbf{m}\mathrm{d}\mathbf{q}\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}\ \mathrm{e}^{N\Psi(\mathbf{m},\mathbf{q},\hat{\mathbf{m}},\hat{\mathbf{q}})}\end{aligned}$$

- Since $\overline{F} = \mathcal{O}(N)$,
  large N behaviour follows from

$$\overline{f} = \lim_{N\to\infty}\overline{F}/N = \lim_{N\to\infty}\lim_{n\to 0}\frac{1}{nN}\log\int \mathrm{d}\mathbf{m}\mathrm{d}\mathbf{q}\mathrm{d}\hat{\mathbf{m}}\mathrm{d}\hat{\mathbf{q}}\ \mathrm{e}^{N\Psi(\mathbf{m},\mathbf{q},\hat{\mathbf{m}},\hat{\mathbf{q}})}$$

- assume limits commute,
  steepest descent integration: $\overline{f} = \lim_{n\to 0}\frac{1}{n}\mathrm{extr}_{\mathbf{m},\mathbf{q},\hat{\mathbf{m}},\hat{\mathbf{q}}}\Psi(\mathbf{m},\mathbf{q},\hat{\mathbf{m}},\hat{\mathbf{q}})$

$$\Psi(\ldots) = \frac{1}{2}\beta J_0 \sum_\alpha m_\alpha^2 + \frac{1}{4}(\beta J)^2 \sum_{\alpha\gamma} q_{\alpha\gamma}^2 + \mathrm{i}\sum_\alpha \hat{m}_\alpha m_\alpha + \mathrm{i}\sum_{\alpha\gamma} \hat{q}_{\alpha\gamma} q_{\alpha\gamma} + \log\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\mathrm{i}\sum_\lambda \hat{m}_\lambda \sigma_\lambda - \mathrm{i}\sum_{\lambda\zeta} \sigma_\lambda \hat{q}_{\lambda\zeta}\sigma_\zeta}$$

- **saddle-point eqns**

$$\frac{\partial\Psi}{\partial m_\alpha} = 0,\ \frac{\partial\Psi}{\partial q_{\alpha\gamma}} = 0: \quad \beta J_0 m_\alpha + \mathrm{i}\hat{m}_\alpha = 0, \quad \frac{1}{2}(\beta J)^2 q_{\alpha\gamma} + \mathrm{i}\hat{q}_{\alpha\gamma} = 0$$

$$\frac{\partial\Psi}{\partial \hat{m}_\alpha} = 0: \quad \mathrm{i}m_\alpha - \mathrm{i}\frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \mathrm{e}^{-\mathrm{i}\sum_\lambda \hat{m}_\lambda \sigma_\lambda - \mathrm{i}\sum_{\lambda\zeta} \sigma_\lambda \hat{q}_{\lambda\zeta}\sigma_\zeta}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\mathrm{i}\sum_\lambda \hat{m}_\lambda \sigma_\lambda - \mathrm{i}\sum_{\lambda\zeta} \sigma_\lambda \hat{q}_{\lambda\zeta}\sigma_\zeta}} = 0$$

$$\frac{\partial\Psi}{\partial \hat{q}_{\alpha\gamma}} = 0: \quad \mathrm{i}q_{\alpha\gamma} - \mathrm{i}\frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha\sigma_\gamma \mathrm{e}^{-\mathrm{i}\sum_\lambda \hat{m}_\lambda \sigma_\lambda - \mathrm{i}\sum_{\lambda\zeta} \sigma_\lambda \hat{q}_{\lambda\zeta}\sigma_\zeta}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\mathrm{i}\sum_\lambda \hat{m}_\lambda \sigma_\lambda - \mathrm{i}\sum_{\lambda\zeta} \sigma_\lambda \hat{q}_{\lambda\zeta}\sigma_\zeta}} = 0$$

- **eliminate $(\hat{\mathbf{m}}, \hat{\mathbf{q}})$**

$$m_\alpha = \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \mathrm{e}^{\beta J_0 \sum_\lambda m_\lambda\sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda\neq\zeta} \sigma_\lambda q_{\lambda\zeta}\sigma_\zeta}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{\beta J_0 \sum_\lambda m_\lambda\sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda\neq\zeta} \sigma_\lambda q_{\lambda\zeta}\sigma_\zeta}}$$

$$q_{\alpha\gamma} = \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha\sigma_\gamma \mathrm{e}^{\beta J_0 \sum_\lambda m_\lambda\sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda\neq\zeta} \sigma_\lambda q_{\lambda\zeta}\sigma_\zeta}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{\beta J_0 \sum_\lambda m_\lambda\sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda\neq\zeta} \sigma_\lambda q_{\lambda\zeta}\sigma_\zeta}}$$

trivial soln: $\mathbf{m}=\mathbf{q}=\mathbf{0}$*, any others?*

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Replica symmetry

- $\beta = 0$ (infinite noise level):

$$m_\alpha = \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha e^0}{\sum_{\boldsymbol{\sigma}} e^0} = 0, \qquad q_{\alpha\gamma} = \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \sigma_\gamma e^0}{\sum_{\boldsymbol{\sigma}} e^0} = 0 \qquad \mathbf{m} = \mathbf{q} = \mathbf{0} \;\; \textit{if} \;\; \beta = 0$$

- bifurcations from trivial soln:

$$\begin{aligned} m_\alpha &= \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \left[1 + \beta J_0 \sum_\lambda m_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda \neq \zeta} \sigma_\lambda q_{\lambda\zeta} \sigma_\zeta\right]}{\sum_{\boldsymbol{\sigma}} \left[1 + \beta J_0 \sum_\lambda m_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda \neq \zeta} \sigma_\lambda q_{\lambda\zeta} \sigma_\zeta\right]} + \mathcal{O}(\mathbf{m}, \mathbf{q})^2 \\ &= \frac{2^n \beta J_0 m_\alpha}{2^n} + \ldots = \beta J_0 m_\alpha + \ldots \qquad \mathbf{m} \neq \mathbf{0} \;\; \textit{if} \;\; \beta J_0 > 1 \end{aligned}$$

$$\begin{aligned} q_{\alpha\gamma} &= \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \sigma_\gamma \left[1 + \beta J_0 \sum_\lambda m_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda \neq \zeta} \sigma_\lambda q_{\lambda\zeta} \sigma_\zeta\right]}{\sum_{\boldsymbol{\sigma}} \left[1 + \beta J_0 \sum_\lambda m_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 \sum_{\lambda \neq \zeta} \sigma_\lambda q_{\lambda\zeta} \sigma_\zeta\right]} + \mathcal{O}(\mathbf{m}, \mathbf{q})^2 \\ &= \frac{2^n (\beta J)^2 q_{\alpha\gamma} + \ldots}{2^n} + \ldots = (\beta J)^2 q_{\alpha\gamma} + \ldots \qquad \mathbf{q} \neq \mathbf{0} \;\; \textit{if} \;\; \beta J > 1 \end{aligned}$$

how to find form of nontrivial solns $\{m_\alpha, q_{\alpha\gamma}\}$?
need their physical interpretation!
use alternative form(s) of replica identity:

$$\overline{\langle f(\boldsymbol{\sigma})\rangle} = \lim_{n\to 0}\frac{1}{n}\sum_{\gamma=1}^{n}\sum_{\boldsymbol{\sigma}^1}\ldots\sum_{\boldsymbol{\sigma}^n}\overline{f(\boldsymbol{\sigma}^\gamma)\mathrm{e}^{-\beta\sum_{\alpha=1}^n H(\boldsymbol{\sigma}^\alpha)}}$$

$$\overline{\langle\langle f(\boldsymbol{\sigma},\boldsymbol{\sigma}')\rangle\rangle} = \lim_{n\to 0}\frac{1}{n(n-1)}\sum_{\alpha\neq\gamma=1}^{n}\sum_{\boldsymbol{\sigma}^1}\ldots\sum_{\boldsymbol{\sigma}^n}\overline{f(\boldsymbol{\sigma}^\alpha,\boldsymbol{\sigma}^\gamma)\mathrm{e}^{-\beta\sum_{\alpha=1}^n H(\boldsymbol{\sigma}^\alpha)}}$$

apply to

$$P(m|\boldsymbol{\sigma}) = \delta\Big[m - \frac{1}{N}\sum_{i=1}^{N}\xi_i\sigma_i\Big], \qquad P(q|\boldsymbol{\sigma},\boldsymbol{\sigma}') = \delta\Big[q - \frac{1}{N}\sum_{i=1}^{N}\sigma_i\sigma_i'\Big]$$

repeat steps of previous calculation,
gives expressions in terms of
saddle-point soln $\{m_\alpha, q_{\alpha\gamma}\}$:

$$\lim_{N\to\infty}\overline{\langle P(m|\boldsymbol{\sigma})\rangle} = \lim_{n\to 0}\frac{1}{n}\sum_{\alpha=1}^{n}\delta[m-m_\alpha]$$

$$\lim_{N\to\infty}\overline{\langle\langle P(q|\boldsymbol{\sigma},\boldsymbol{\sigma}')\rangle\rangle} = \lim_{n\to 0}\frac{1}{n(n-1)}\sum_{\alpha\neq\gamma=1}^{n}\delta[q-q_{\alpha\gamma}]$$

ergodic mean-field systems

fluctuations in quantities like $\frac{1}{N}\sum_{i=1}^N \xi_i\sigma_i$
or $\frac{1}{N}\sum_{i=1}^N \sigma_i\sigma_i'$ scale as $\mathcal{O}(N^{-1/2})$

hence

$$\lim_{N\to\infty}\langle P(m|\boldsymbol{\sigma})\rangle = \lim_{N\to\infty}\Big\langle \delta\Big[m-\frac{1}{N}\sum_{i=1}^N \xi_i\sigma_i\Big]\Big\rangle = \delta\Big[m-\frac{1}{N}\sum_{i=1}^N \xi_i\langle\sigma_i\rangle\Big]$$

$$\lim_{N\to\infty}\langle\langle P(q|\boldsymbol{\sigma},\boldsymbol{\sigma}')\rangle\rangle = \lim_{N\to\infty}\Big\langle\Big\langle \delta\Big[q-\frac{1}{N}\sum_{i=1}^N \sigma_i\sigma_i'\Big]\Big\rangle\Big\rangle = \delta\Big[q-\frac{1}{N}\sum_{i=1}^N \langle\sigma_i\rangle^2\Big]$$

hence

$$\forall\alpha: \qquad m_\alpha = m = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^N \xi_i\overline{\langle\sigma_i\rangle}$$

$$\forall\alpha\neq\gamma: \qquad q_{\alpha\gamma} = q = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^N \overline{\langle\sigma_i\rangle^2}$$

replica-symmetric solution

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Replica symmetric solution

$m_\alpha = m,\;\; q_{\alpha\neq\beta} = q,$ now find m and q ...

- **RS saddle-point eqns**
  insert RS form and use $\exp(\frac{1}{2}x^2) = \int \mathrm{D}z\; \mathrm{e}^{xz}$

$$
\begin{aligned}
m &= \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \mathrm{e}^{\beta J_0 m \sum_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 q \sum_{\lambda\neq\zeta} \sigma_\lambda \sigma_\zeta}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{\beta J_0 m \sum_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 q \sum_{\lambda\neq\zeta} \sigma_\lambda \sigma_\zeta}} = \frac{\sum_{\boldsymbol{\sigma}} \sigma_\alpha \mathrm{e}^{\beta J_0 m \sum_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 q [\sum_\lambda \sigma_\lambda]^2}}{\sum_{\boldsymbol{\sigma}} \mathrm{e}^{\beta J_0 m \sum_\lambda \sigma_\lambda + \frac{1}{2}(\beta J)^2 q [\sum_\lambda \sigma_\lambda]^2}} \\
&= \frac{\int \mathrm{D}z \sum_{\boldsymbol{\sigma}} \sigma_\alpha \prod_{\lambda=1}^{n} \mathrm{e}^{\beta(J_0 m + Jz\sqrt{q})\sigma_\lambda}}{\int \mathrm{D}z \sum_{\boldsymbol{\sigma}} \prod_{\lambda=1}^{n} \mathrm{e}^{\beta(J_0 m + Jz\sqrt{q})\sigma_\lambda}} \\
&= \frac{\int \mathrm{D}z\; \sinh[\beta(J_0 m + Jz\sqrt{q})] \cosh^{n-1}[\beta(J_0 m + Jz\sqrt{q})]}{\int \mathrm{D}z\; \cosh^{n}[\beta(J_0 m + Jz\sqrt{q})]}
\end{aligned}
$$

similarly

$$
q = \frac{\int \mathrm{D}z\; \sinh^2[\beta(J_0 m + Jz\sqrt{q})] \cosh^{n-2}[\beta(J_0 m + Jz\sqrt{q})]}{\int \mathrm{D}z\; \cosh^{n}[\beta(J_0 m + Jz\sqrt{q})]}
$$

- **the limit** $n \to 0$

$$
m = \int \mathrm{D}z\; \tanh[\beta(J_0 m + Jz\sqrt{q})], \qquad q = \int \mathrm{D}z\; \tanh^2[\beta(J_0 m + Jz\sqrt{q})]
$$

RS equations for $m = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \xi_i \overline{\langle\sigma_i\rangle}$
and $q = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \overline{\langle\sigma_i\rangle^2}$

$$m = \int \mathrm{D}z\ \tanh[\beta(J_0 m + Jz\sqrt{q})], \qquad q = \int \mathrm{D}z\ \tanh^2[\beta(J_0 m + Jz\sqrt{q})]$$

- bifurcations away from $(m,q) = (0,0)$:

$$\begin{aligned} m &= \int \mathrm{D}z\ \left[\beta J_0 m + \beta Jz\sqrt{q} + \mathcal{O}(m,\sqrt{q})^3\right] = \beta J_0 m + \ldots \\ q &= \int \mathrm{D}z\ \left[\beta J_0 m + \beta Jz\sqrt{q} + \mathcal{O}(m,\sqrt{q})^3\right]^2 = \int \mathrm{D}z\ (\beta J)^2 z^2 q + \ldots \\ &= (\beta J)^2 q + \ldots \end{aligned}$$

hence:
first continuous bifurcations away from $\mathbf{q} = \mathbf{m} = \mathbf{0}$,
as identified earlier, are the RS solutions

$$m = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \xi_i \overline{\langle\sigma_i\rangle}, \qquad q = \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} \overline{\langle\sigma_i\rangle^2}$$

$$m = \int \mathrm{D}z\ \tanh[\beta(J_0 m + Jz\sqrt{q})], \qquad q = \int \mathrm{D}z\ \tanh^2[\beta(J_0 m + Jz\sqrt{q})]$$

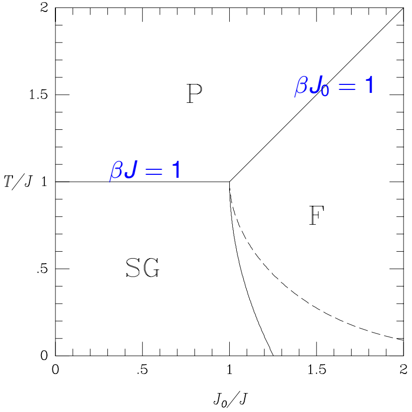
phase diagram

P: $m = q = 0$
random neuronal firing

SG: $m = 0$, $q > 0$
stable firing patterns, but
not related to stored pattern

F: $m, q > 0$
recall of stored information

$T = 1/\beta$ (noise strength)



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Linear separability of data and version space

Dimension mismatch and overfitting

two clinical outcomes (A,B),
4 patients, 60 expression levels ...

A : (100101001010010101010010001010111001001001001001000011111)
A : (010001000010101001010101010010101000111100101001001010101000)
B : (001010001110101101100100100111001110010100101010101000101010)
B : (101011001010110010100100111100100101100111010111010001010010)

prognostic signature!

A : (100101001010010101010010001010111001001001001001000011111)
A : (010001000010101001010101010010101000111100101001001010101000)
B : (001010001110101101100100100111001110010100101010101000101010)
B : (101011001010110010100100111100100101100111010111010001010010)

shuffle outcome labels ...

A : (100101001010010101010010001010111001001001001001000011111)
B : (010001000010101001010101010010101000111100101001001010101000)
A : (001010001110101101100100100111001110010100101010101000101010)
B : (101011001010110010100100111100100101100111010111010001010010)

overfitting, no reproducibility ...
how about overfitting in regression?

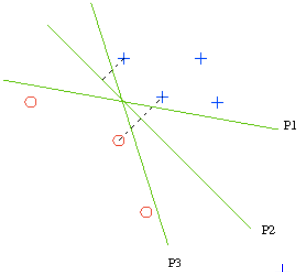
Suppose we have data D on N patients,
pairs of covariate vectors + clinical outcome labels

$$D = \{(\mathbf{x}^1, t^1), \ldots, (\mathbf{x}^N, t^N)\}, \qquad \mathbf{x}^i \in \{-1,1\}^p, \quad t^i \in \{-1,1\}, \qquad p, N \gg 1$$

e.g. $\mathbf{x}^i$= gene expressions of i (on/off)
t^i= treatment response of i (yes/no)

- assumed model:

$$t(\mathbf{x}) = \begin{cases} 1 & \text{if } \sum_{\mu=1}^p \theta_\mu x_\mu > 0 \\ -1 & \text{if } \sum_{\mu=1}^p \theta_\mu x_\mu < 0 \end{cases}$$
$$= sgn\Big[\sum_{\mu=1}^p \theta_\mu x_\mu\Big]$$



$+$: $t^i = 1$
o : $t^i = -1$

- regression/classification task:
find parameters $\boldsymbol{\theta} = (\theta_1 \ldots, \theta_p)$
such that

$$\textit{for all } i = 1 \ldots N: \qquad t^i = sgn\Big[\sum_{\mu=1}^p \theta_\mu x^i_\mu\Big]$$

- data D explained perfectly by $\boldsymbol{\theta}$ if

$$\textit{for all } i=1\ldots N: \qquad t^i = sgn[\boldsymbol{\theta}\cdot\mathbf{x}^i], \quad \textit{i.e.} \quad t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)>0$$

$$\textit{separating plane in input space}: \qquad \boldsymbol{\theta}\cdot\mathbf{x}=0$$

$$\textit{distance } \Delta_i \textit{ between } \mathbf{x}^i \textit{ and separating plane}: \qquad d_i = t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)/|\boldsymbol{\theta}|$$

$$|\boldsymbol{\theta}| \textit{ irrelevant}, \textit{ so choose } |\boldsymbol{\theta}|^2 = p$$

- **version space**

  all $\boldsymbol{\theta}$ that solve above eqns
  with distances κ or larger

  volume of version space:

$$V(\kappa) = \int \mathrm{d}\boldsymbol{\theta}\ \delta(\boldsymbol{\theta}^2-p)\prod_{i=1}^N \theta\Big[\frac{t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)}{\sqrt{p}}>\kappa\Big]$$

- high dimensional data: p large, $\alpha=N/p$
  $V(\kappa)$ scales exponentially with p, so

$$F = \frac{1}{p}\log V(\kappa) = \frac{1}{p}\log\int \mathrm{d}\boldsymbol{\theta}\ \delta(\boldsymbol{\theta}^2-p)\prod_{i=1}^N \theta\Big[\frac{t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)}{\sqrt{p}}>\kappa\Big]$$

$F=-\infty$: no solutions $\boldsymbol{\theta}$ exist, data D not linearly separable
$F=$ finite: solutions $\boldsymbol{\theta}$ exist, data D linearly separable

overfitting: find parameters $\boldsymbol{\theta}$ that 'explain' random patterns
what if we choose **random data** D?

$$D=\{(\mathbf{x}^1,t^1),\ldots,(\mathbf{x}^N,t^N)\},\qquad \mathbf{x}^i\in\{-1,1\}^p,\;\; t^i\in\{-1,1\},\;\; \textit{fully random}$$

typical classification performance:

$$\begin{aligned}\overline{F} &= \overline{\frac{1}{p}\log\int\!\mathrm{d}\boldsymbol{\theta}\;\delta(p-\boldsymbol{\theta}^2)\prod_{i=1}^N\theta\Big[\frac{t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)}{\sqrt{p}}>\kappa\Big]} \\ &= \overline{\frac{1}{p}\log\int\!\frac{\mathrm{d}z}{2\pi}\mathrm{e}^{\mathrm{i}zp}\int\!\mathrm{d}\boldsymbol{\theta}\;\mathrm{e}^{-\mathrm{i}z\boldsymbol{\theta}^2}\prod_{i=1}^N\theta\Big[\frac{t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)}{\sqrt{p}}>\kappa\Big]}\end{aligned}$$

transport data vars to harmless place,
using δ-functions, by inserting

$$1=\int\!\mathrm{d}y_i\;\delta\Big[y_i-\frac{t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)}{\sqrt{p}}\Big]=\int\!\frac{\mathrm{d}y_i\mathrm{d}\hat{y}_i}{2\pi}\;\mathrm{e}^{\mathrm{i}\hat{y}_iy_i-\mathrm{i}\hat{y}_it^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)/\sqrt{p}}$$

gives

$$\overline{F}=\overline{\frac{1}{p}\log\int\!\frac{\mathrm{d}z\mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\mathrm{d}\boldsymbol{\theta}}{(2\pi)^{N+1}}\mathrm{e}^{\mathrm{i}zp+\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}-\mathrm{i}z\boldsymbol{\theta}^2}\Big(\prod_{i=1}^N\theta(y_i-\kappa)\mathrm{e}^{-\mathrm{i}\hat{y}_it^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)/\sqrt{p}}\Big)}$$

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The replica calculation

large p, large N,
$N = \alpha p$:

$$\overline{F} = \lim_{p\to\infty} \frac{1}{p} \overline{\log \int \frac{\mathrm{d}z\mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\mathrm{d}\boldsymbol{\theta}}{(2\pi)^{N+1}} \mathrm{e}^{\mathrm{i}zp+\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}-\mathrm{i}z\boldsymbol{\theta}^2} \Big(\prod_{i=1}^{N} \theta(y_i-\kappa)\mathrm{e}^{-\mathrm{i}\hat{y}_i t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)/\sqrt{p}}\Big)}$$

- **replica identity**

  $\overline{\log Z} = \lim_{n\to 0} n^{-1} \log \overline{Z^n}$

$$\overline{F} = \lim_{p\to\infty} \lim_{n\to 0} \frac{1}{pn} \log \overline{\Big[\int \frac{\mathrm{d}z\mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\mathrm{d}\boldsymbol{\theta}}{(2\pi)^{N+1}} \mathrm{e}^{\mathrm{i}zp+\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}-\mathrm{i}z\boldsymbol{\theta}^2} \Big(\prod_{i=1}^{N} \theta(y_i-\kappa)\mathrm{e}^{-\mathrm{i}\hat{y}_i t^i(\boldsymbol{\theta}\cdot\mathbf{x}^i)/\sqrt{p}}\Big)\Big]^n}$$

$$= \lim_{p\to\infty} \lim_{n\to 0} \frac{1}{pn} \log \int \prod_{\alpha=1}^{n} \Big[\frac{\mathrm{d}z^\alpha\mathrm{d}\mathbf{y}^\alpha\mathrm{d}\hat{\mathbf{y}}^\alpha\mathrm{d}\boldsymbol{\theta}^\alpha}{(2\pi)^{N+1}} \mathrm{e}^{\mathrm{i}pz^\alpha+\mathrm{i}\hat{\mathbf{y}}^\alpha\cdot\mathbf{y}^\alpha-\mathrm{i}z^\alpha(\boldsymbol{\theta}^\alpha)^2} \prod_{i=1}^{N} \theta[y_i^\alpha-\kappa]\Big] \times \overline{\mathrm{e}^{-\mathrm{i}\sum_{i=1}^{N}\sum_{\alpha=1}^{n} \hat{y}_i^\alpha t^i(\boldsymbol{\theta}^\alpha\cdot\mathbf{x}^i)/\sqrt{p}}}$$

- **average over data D:**

$$
\begin{aligned}
\Xi &= \overline{e^{-i\sum_{i=1}^{N}\sum_{\alpha=1}^{n}\hat{y}_i^\alpha t^i(\boldsymbol{\theta}^\alpha\cdot\mathbf{x}^i)/\sqrt{p}}} = \overline{e^{-i\sum_{\mu=1}^{p}\sum_{i=1}^{N} t^i x_\mu^i \sum_{\alpha=1}^{n}\hat{y}_i^\alpha\theta_\mu^\alpha/\sqrt{p}}} \\
&= \prod_{\mu=1}^{p}\prod_{i=1}^{N}\overline{e^{-it^i x_\mu^i\sum_{\alpha=1}^{n}\hat{y}_i^\alpha\theta_\mu^\alpha/\sqrt{p}}} = \prod_{\mu=1}^{p}\sum_{i=1}^{N}\cos\Big[\frac{1}{\sqrt{p}}\sum_{\alpha=1}^{n}\hat{y}_i^\alpha\theta_\mu^\alpha\Big] \\
&= \prod_{\mu=1}^{p}\prod_{i=1}^{N}\Big\{1-\frac{1}{2p}\Big(\sum_{\alpha=1}^{n}\hat{y}_i^\alpha\theta_\mu^\alpha\Big)^2+\mathcal{O}(\frac{1}{p^2})\Big\} = e^{-\frac{1}{2p}\sum_{\mu=1}^{p}\sum_{i=1}^{N}\sum_{\alpha,\beta=1}^{n}\hat{y}_i^\alpha\hat{y}_i^\beta\theta_\mu^\alpha\theta_\mu^\beta+\mathcal{O}(p^0)}
\end{aligned}
$$

- giving

$$
\begin{aligned}
\overline{F} &= \lim_{p\to\infty}\lim_{n\to 0}\frac{1}{pn}\log\int\prod_{\alpha=1}^{n}\Big[\frac{dz^\alpha d\mathbf{y}d\hat{\mathbf{y}}^\alpha d\boldsymbol{\theta}^\alpha}{(2\pi)^{N+1}}e^{ipz^\alpha+i\hat{\mathbf{y}}^\alpha\cdot\mathbf{y}^\alpha-iz(\boldsymbol{\theta}^\alpha)^2}\prod_{i=1}^{N}\theta(y_i^\alpha-\kappa)\Big] \\
&\qquad\qquad\times e^{-\frac{1}{2p}\sum_{\mu=1}^{p}\sum_{i=1}^{N}\sum_{\alpha,\beta=1}^{n}\hat{y}_i^\alpha\hat{y}_i^\beta\theta_\mu^\alpha\theta_\mu^\beta+\mathcal{O}(p^0)} \\
&= -\alpha\log(2\pi)+\lim_{p\to\infty}\lim_{n\to 0}\frac{1}{pn}\log\int\prod_{\alpha=1}^{n}\Big(dz^\alpha d\boldsymbol{\theta}^\alpha e^{ipz^\alpha-z^\alpha(\boldsymbol{\theta}^\alpha)^2}\Big) \\
&\quad\times\prod_{i=1}^{N}\int\prod_{\alpha=1}^{n}\Big[dy_i^\alpha d\hat{y}_i^\alpha e^{i\sum_\alpha\hat{y}_i^\alpha y_i^\alpha}\theta[y_i^\alpha-\kappa]\Big]e^{-\frac{1}{2}\sum_{\alpha,\beta}\hat{y}_i^\alpha\hat{y}_i^\beta[\frac{1}{p}\sum_{\mu=1}^{p}\theta_\mu^\alpha\theta_\mu^\beta]}
\end{aligned}
$$

- so, with $\mathbf{y}=(y_1,\ldots,y_n)$, $\hat{\mathbf{y}}=(\hat{y}_1,\ldots,\hat{y}_n)$, $\mathbf{z}=(z_1,\ldots,z_n)$:

$$\overline{F} = -\alpha\log(2\pi)+\lim_{p\to\infty}\lim_{n\to 0}\frac{1}{pn}\log\int \mathrm{d}\mathbf{z}\Big(\prod_{\alpha=1}^{n}\mathrm{d}\boldsymbol{\theta}^{\alpha}\,\mathrm{e}^{\mathrm{i}pz^{\alpha}-z^{\alpha}(\boldsymbol{\theta}^{\alpha})^2}\Big) \times\Big\{\int \mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\;\mathrm{e}^{\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}}\prod_{\alpha=1}^{n}\theta[y^{\alpha}-\kappa]\;\mathrm{e}^{-\frac{1}{2}\sum_{\alpha,\beta}\hat{y}^{\alpha}\hat{y}^{\beta}[\frac{1}{p}\sum_{\mu=1}^{p}\theta_{\mu}^{\alpha}\theta_{\mu}^{\beta}]}\Big\}^{N}$$

- insert

$$1=\int \mathrm{d}q_{\alpha\beta}\;\delta\Big[q_{\alpha\beta}-\frac{1}{p}\sum_{\mu=1}^{p}\theta_{\mu}^{\alpha}\theta_{\mu}^{\beta}\Big]=\int\frac{\mathrm{d}q_{\alpha\beta}\mathrm{d}\hat{q}_{\alpha\beta}}{2\pi/p}\;\mathrm{e}^{\mathrm{i}p\hat{q}_{\alpha\beta}\left[q_{\alpha\beta}-\frac{1}{p}\sum_{\mu=1}^{p}\theta_{\mu}^{\alpha}\theta_{\mu}^{\beta}\right]}$$

to get

$$\overline{F} = -\alpha\log(2\pi)+\lim_{p\to\infty}\lim_{n\to 0}\frac{1}{pn}\log\int \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{q}\mathrm{d}\hat{\mathbf{q}}\;\mathrm{e}^{\mathrm{i}p\sum_{\alpha\beta=1}^{n}\hat{q}_{\alpha\beta}q_{\alpha\beta}+\mathrm{i}p\sum_{\alpha=1}^{n}z_{\alpha}} \times\Big\{\int \mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\;\mathrm{e}^{\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}}\prod_{\alpha=1}^{n}\theta[y^{\alpha}-\kappa]\;\mathrm{e}^{-\frac{1}{2}\hat{\mathbf{y}}\cdot\mathbf{q}\hat{\mathbf{y}}}\Big\}^{N}\int\prod_{\alpha=1}^{n}\Big(\mathrm{d}\boldsymbol{\theta}^{\alpha}\mathrm{e}^{-\mathrm{i}z^{\alpha}(\boldsymbol{\theta}^{\alpha})^2}\Big)\mathrm{e}^{-\mathrm{i}\sum_{\mu=1}^{p}\sum_{\alpha\beta}\hat{q}_{\alpha\beta}\theta_{\mu}^{\alpha}\theta_{\mu}^{\beta}}$$

- so, with $\boldsymbol{\theta}=(\theta_1,\ldots,\theta_n)$:
(remember: $N=\alpha p$)

$$\begin{aligned}
\overline{F} &= -\alpha\log(2\pi)+\lim_{p\to\infty}\lim_{n\to 0}\frac{1}{pn}\log\int \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{q}\mathrm{d}\hat{\mathbf{q}}\ \mathrm{e}^{\mathrm{i}p\sum_{\alpha\beta=1}^{n}\hat{q}_{\alpha\beta}q_{\alpha\beta}+\mathrm{i}p\sum_{\alpha=1}^{n}z_\alpha} \\
&\quad\times\Big\{\int \mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\ \mathrm{e}^{\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}}\prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\ \mathrm{e}^{-\frac{1}{2}\hat{\mathbf{y}}\cdot\mathbf{q}\hat{\mathbf{y}}}\Big\}^{\alpha p}\Big\{\int \mathrm{d}\boldsymbol{\theta}\ \mathrm{e}^{-\mathrm{i}\sum_{\alpha=1}^{n}z^\alpha\theta_\alpha^2-\mathrm{i}\boldsymbol{\theta}\cdot\hat{\mathbf{q}}\boldsymbol{\theta}}\Big\}^{p} \\
&= \lim_{p\to\infty}\lim_{n\to 0}\frac{1}{pn}\log\int \mathrm{d}\mathbf{z}\mathrm{d}\mathbf{q}\mathrm{d}\hat{\mathbf{q}}\ \mathrm{e}^{p\Psi(\mathbf{z},\mathbf{q},\hat{\mathbf{q}})} \\
\Psi(\ldots) &= \mathrm{i}\sum_{\alpha\beta=1}^{n}\hat{q}_{\alpha\beta}q_{\alpha\beta}+\mathrm{i}\sum_{\alpha=1}^{n}z_\alpha+\log\int \mathrm{d}\boldsymbol{\theta}\ \mathrm{e}^{-\mathrm{i}\sum_{\alpha=1}^{n}z^\alpha\theta_\alpha^2-\mathrm{i}\boldsymbol{\theta}\cdot\hat{\mathbf{q}}\boldsymbol{\theta}} \\
&\quad+\alpha\log\int \mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\ \mathrm{e}^{\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}}\prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\ \mathrm{e}^{-\frac{1}{2}\hat{\mathbf{y}}\cdot\mathbf{q}\hat{\mathbf{y}}}-\alpha n\log(2\pi)
\end{aligned}$$

- assume limits $n\to 0$ and $p\to\infty$ commute,
steepest descent integration

$$\overline{F} = \lim_{n\to 0}\frac{1}{n}\mathrm{extr}_{\mathbf{z},\mathbf{q},\hat{\mathbf{q}}}\Psi(\mathbf{z},\mathbf{q},\hat{\mathbf{q}})$$

$$\begin{aligned}\Psi(\mathbf{z},\mathbf{q},\hat{\mathbf{q}}) &= \mathrm{i}\sum_{\alpha\beta=1}^{n}\hat{q}_{\alpha\beta}q_{\alpha\beta}+\mathrm{i}\sum_{\alpha=1}^{n}z_\alpha+\log\int \mathrm{d}\boldsymbol{\theta}\ \mathrm{e}^{-\mathrm{i}\sum_{\alpha=1}^{n}z^\alpha\theta_\alpha^2-\mathrm{i}\boldsymbol{\theta}\cdot\hat{\mathbf{q}}\boldsymbol{\theta}} \\ &\quad +\alpha\log\int \mathrm{d}\mathbf{y}\mathrm{d}\hat{\mathbf{y}}\ \mathrm{e}^{\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}}\prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\ \mathrm{e}^{-\frac{1}{2}\hat{\mathbf{y}}\cdot\mathbf{q}\hat{\mathbf{y}}}-\alpha n\log(2\pi)\end{aligned}$$

- transform $\hat{q}_{\alpha\beta}=-\frac{1}{2}\mathrm{i}k_{\alpha\beta}-z_\alpha\delta_{\alpha\beta}$, and integrate over $\hat{\mathbf{y}}$:

$$\begin{aligned}\Psi(\mathbf{z},\mathbf{q},\mathbf{k}) &= \frac{1}{2}\sum_{\alpha\beta=1}^{n}k_{\alpha\beta}q_{\alpha\beta}+\mathrm{i}\sum_{\alpha=1}^{n}z_\alpha(1-q_{\alpha\alpha})+\log\int \mathrm{d}\boldsymbol{\theta}\ \mathrm{e}^{-\frac{1}{2}\boldsymbol{\theta}\cdot\mathbf{k}\boldsymbol{\theta}} \\ &\quad +\alpha\log\int \mathrm{d}\mathbf{y}\ \prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\int \mathrm{d}\hat{\mathbf{y}}\ \mathrm{e}^{\mathrm{i}\hat{\mathbf{y}}\cdot\mathbf{y}-\frac{1}{2}\hat{\mathbf{y}}\cdot\mathbf{q}\hat{\mathbf{y}}}-\alpha n\log(2\pi) \\ &= \frac{1}{2}\sum_{\alpha\beta=1}^{n}k_{\alpha\beta}q_{\alpha\beta}+\mathrm{i}\sum_{\alpha=1}^{n}z_\alpha(1-q_{\alpha\alpha})+\log\frac{(2\pi)^{n/2}}{\sqrt{\mathrm{Det}\mathbf{k}}} \\ &\quad +\alpha\log\int \mathrm{d}\mathbf{y}\ \prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\int \mathrm{d}\hat{\mathbf{y}}\ \frac{(2\pi)^{n/2}}{\sqrt{\mathrm{Det}\mathbf{q}}}\mathrm{e}^{-\frac{1}{2}\mathbf{y}\cdot\mathbf{q}^{-1}\mathbf{y}}-\alpha n\log(2\pi)\end{aligned}$$

- re-organise:

$$\Psi(\mathbf{z},\mathbf{q},\mathbf{k}) = \frac{1}{2}\sum_{\alpha\beta=1}^{n} k_{\alpha\beta}q_{\alpha\beta} + \mathrm{i}\sum_{\alpha=1}^{n} z_\alpha(1-q_{\alpha\alpha}) - \frac{1}{2}\log\mathrm{Det}\,\mathbf{k} - \frac{1}{2}\alpha\log\mathrm{Det}\,\mathbf{q}$$
$$+\alpha\log\int\mathrm{d}\mathbf{y}\,\prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\mathrm{e}^{-\frac{1}{2}\mathbf{y}\cdot\mathbf{q}^{-1}\mathbf{y}} + \frac{1}{2}n(1-\alpha)\log(2\pi)$$

- extremise with respect to $\mathbf{z}$:
$\partial\Psi/\partial z_\alpha = 0: \quad q_{\alpha\alpha} = 0$ for all α

$$\Psi(\mathbf{q},\mathbf{k}) = \frac{1}{2}n(1-\alpha)\log(2\pi) + \frac{1}{2}\sum_{\alpha\beta=1}^{n} k_{\alpha\beta}q_{\alpha\beta} - \frac{1}{2}\log\mathrm{Det}\,\mathbf{k} - \frac{1}{2}\alpha\log\mathrm{Det}\,\mathbf{q}$$
$$+\alpha\log\int\mathrm{d}\mathbf{y}\,\prod_{\alpha=1}^{n}\theta[y^\alpha-\kappa]\mathrm{e}^{-\frac{1}{2}\mathbf{y}\cdot\mathbf{q}^{-1}\mathbf{y}}$$

next: ergodicity assumption,
replica-symmetric form for **q** and **k** ...

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   - **Gardner's replica symmetric theory**
   - Overfitting transition in Cox regression

Gardner's replica symmetric theory

$$\Psi(\mathbf{q},\mathbf{k}) = \frac{1}{2}n(1-\alpha)\log(2\pi) + \frac{1}{2}\sum_{\alpha\beta=1}^{n} k_{\alpha\beta}q_{\alpha\beta} - \frac{1}{2}\log \mathrm{Det}\,\mathbf{k} - \frac{1}{2}\alpha\log \mathrm{Det}\,\mathbf{q}$$
$$+\alpha\log\int \mathrm{d}\mathbf{y}\,\prod_{\alpha=1}^{n}\theta[y^{\alpha}-\kappa]\mathrm{e}^{-\frac{1}{2}\mathbf{y}\cdot\mathbf{q}^{-1}\mathbf{y}}$$

RS saddle-points

$$q_{\alpha\beta} = \delta_{\alpha\beta} + (1-\delta_{\alpha\beta})q, \qquad k_{\alpha\beta} = K\delta_{\alpha\beta} + (1-\delta_{\alpha\beta})k$$

- eigenvalues:

$$\mathbf{x} = (1,\ldots,1): \qquad (\mathbf{kx})_{\alpha} = \sum_{\beta=1}^{n}[k+(K-k)\delta_{\alpha\beta}]x_{\beta} = nk+K-k$$
$$\textit{eigenvalue}: \quad \lambda = nk+K-k$$

$$\sum_{\alpha=1}^{n}x_{\alpha} = 0: \qquad (\mathbf{kx})_{\alpha} = \sum_{\beta=1}^{n}[k+(K-k)\delta_{\alpha\beta}]x_{\beta} = (K-k)x_{\alpha}$$
$$\textit{eigenvalue}: \quad \lambda = K-k \quad (n-1\ \textit{fold})$$

hence

$$\mathrm{Det}\,\mathbf{k} = (nk+K-k)(K-k)^{n-1}, \qquad \mathrm{Det}\,\mathbf{q} = (nq+1-q)(1-q)^{n-1}$$

- invert $\mathbf{q}$, try $(\mathbf{q}^{-1})_{\alpha\beta} = r + (R-r)\delta_{\alpha\beta}$, demand:

$$\begin{aligned}\delta_{\alpha\beta} &= (\mathbf{q}\mathbf{q}^{-1})_{\alpha\beta} = \sum_{\gamma}(q+(1-q)\delta_{\alpha\gamma})(r+(R-r)\delta_{\gamma\beta}) \\ &= nqr + q(R-r) + r(1-q) + (R-r)(1-q)\delta_{\alpha\beta}\end{aligned}$$

so
$$nqr + q(R-r) + r(1-q) = 0, \qquad (R-r)(1-q) = 1$$
$$R = r + \frac{1}{1-q}, \qquad r = -\frac{q}{(1-q)(1-q+nq)}$$

- hence, using $\exp[\frac{1}{2}x^2] = \int \mathrm{D}z\ \mathrm{e}^{xz}$

$$\begin{aligned}\log \int \mathrm{d}\mathbf{y} \prod_{\alpha=1}^{n} \theta[y^\alpha - \kappa]\mathrm{e}^{-\frac{1}{2}\mathbf{y}\cdot\mathbf{q}^{-1}\mathbf{y}} &= \log \int \mathrm{d}\mathbf{y} \prod_{\alpha=1}^{n} \theta[y^\alpha - \kappa]\mathrm{e}^{-\frac{1}{2}\sum_{\alpha\beta} y_\alpha[r+(R-r)\delta_{\alpha\beta}]y_\beta} \\ &= \log \int \mathrm{d}\mathbf{y} \prod_{\alpha=1}^{n} \theta[y^\alpha - \kappa]\mathrm{e}^{-\frac{1}{2}r[\sum_{\alpha\beta} y_\alpha]^2 - \frac{1}{2}(R-r)\sum_\alpha y_\alpha^2} \\ &= \log \int \mathrm{D}z \int \mathrm{d}\mathbf{y} \prod_{\alpha=1}^{n} \theta[y^\alpha - \kappa]\mathrm{e}^{z\sqrt{-r}\sum_{\alpha\beta} y_\alpha - \frac{1}{2}(R-r)\sum_\alpha y_\alpha^2} \\ &= \log \int \mathrm{D}z \Big[\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{z\sqrt{-r}y - \frac{1}{2}(R-r)y^2}\Big]^n\end{aligned}$$

put everything together ...

$$
\begin{aligned}
\frac{1}{n}\Psi(\mathbf{q},\mathbf{k}) &= \frac{1}{2}(1-\alpha)\log(2\pi)+\frac{1}{2}K+\frac{1}{2}(n-1)qk-\frac{1}{2n}\log[(nk+K-k)(K-k)^{n-1}] \\
&\quad -\frac{\alpha}{2n}\log[(nq+1-q)(1-q)^{n-1}]+\frac{\alpha}{n}\log\int \mathrm{D}z\Big[\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{z\sqrt{-r}y-\frac{1}{2}(R-r)y^2}\Big]^n \\
&= \frac{1}{2}(1-\alpha)\log(2\pi)+\frac{1}{2}(K-qk)-\frac{1}{2n}\log(1+\frac{nk}{K-k})-\frac{1}{2}\log(K-k) \\
&\quad -\frac{\alpha}{2n}\log(1+\frac{nq}{1-q})-\frac{\alpha}{2}\log(1-q)+\mathcal{O}(n) \\
&\quad +\frac{\alpha}{n}\log\int \mathrm{D}z\Big[1+n\log\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{zy\sqrt{q}/(1-q)-\frac{1}{2(1-q)}y^2}+\mathcal{O}(n^2)\Big]
\end{aligned}
$$

take limit $n\to 0$:

$$
\begin{aligned}
2\overline{F} &= (1-\alpha)\log(2\pi)+\mathrm{extr}_{K,k,q}\Big\{K-qk-\frac{k}{K-k}-\log(K-k) \\
&\quad -\frac{\alpha q}{1-q}-\alpha\log(1-q)+2\alpha\int \mathrm{D}z\ \log\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{zy\sqrt{q}/(1-q)-\frac{1}{2(1-q)}y^2}\Big\}
\end{aligned}
$$

$$
\begin{aligned}
2\overline{F} &= (1-\alpha)\log(2\pi) + \mathrm{extr}_{K,k,q}\Big\{K - qk - \frac{k}{K-k} - \log(K-k) \\
&\quad - \frac{\alpha q}{1-q} - \alpha\log(1-q) + 2\alpha\int \mathrm{D}z\ \log\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{zy\sqrt{q}/(1-q)-\frac{1}{2(1-q)}y^2}\Big\}
\end{aligned}
$$

- **extremise over K and k**

$$
\left\{\begin{array}{ll}
\frac{\partial}{\partial K}=0: & 1+\frac{k}{(K-k)^2}-\frac{1}{K-k}=0 \\
\frac{\partial}{\partial k}=0: & -q-\frac{1}{K-k}-\frac{k}{(K-k)^2}+\frac{1}{K-k}=0
\end{array}\right.
\Rightarrow\quad K=\frac{1-2q}{(1-q)^2},\quad k=-\frac{q}{(1-q)^2}
$$

result:

$$
\begin{aligned}
2\overline{F} &= (1-\alpha)\log(2\pi) + \mathrm{extr}_q\Big\{\frac{1}{1-q} - \frac{\alpha q}{1-q} + (1-\alpha)\log(1-q) \\
&\quad + 2\alpha\int \mathrm{D}z\ \log\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{zy\sqrt{q}/(1-q)-\frac{1}{2(1-q)}y^2}\Big\}
\end{aligned}
$$

- write y-integral in terms of error function $\mathrm{Erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x \mathrm{d}t\ \mathrm{e}^{-t^2}$:

$$
\begin{aligned}
\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{zy\sqrt{q}/(1-q)-\frac{1}{2(1-q)}y^2} &= \mathrm{e}^{\frac{qz^2}{2(1-q)}}\int_\kappa^\infty \mathrm{d}y\ \mathrm{e}^{-\frac{[y-z\sqrt{q}]^2}{2(1-q)}} \\
&= \sqrt{2(1-q)}\ \mathrm{e}^{\frac{qz^2}{2(1-q)}}\ \frac{\sqrt{\pi}}{2}\Big\{1-\mathrm{Erf}\Big[\frac{K-z\sqrt{q}}{\sqrt{2(1-q)}}\Big]\Big\}
\end{aligned}
$$

- insert previous integral:

$$
\begin{aligned}
2\overline{F} &= \log\pi + (1-2\alpha)\log 2 \\
&\quad + \mathrm{extr}_q\Big\{\frac{1}{1-q} + \log(1-q) + 2\alpha\int \mathrm{D}z\, \log\Big[1-\mathrm{Erf}\Big(\frac{K-z\sqrt{q}}{\sqrt{2(1-q)}}\Big)\Big]\Big\}
\end{aligned}
$$

- **extremisation with respect to q**

short-hand $u(z,q)=(\kappa-z\sqrt{q})/\sqrt{2(1-q)}$,
use $\mathrm{Erf}'(x)=\frac{2}{\sqrt{\pi}}\exp[-x^2]$

$$
\frac{\mathrm{d}}{\mathrm{d}q}=0: \qquad \frac{1}{(1-q)^2}-\frac{1}{1-q}-2\alpha\int \mathrm{D}z\,\Big(\frac{\partial u}{\partial q}\Big)\frac{\mathrm{Erf}'\,u(z,q)}{1-\mathrm{Erf}\,u(z,q)}=0
$$

$$
\frac{q}{(1-q)^2}=\frac{4\alpha}{\sqrt{\pi}}\int \mathrm{D}z\,\Big(\frac{\partial u}{\partial q}\Big)\frac{\mathrm{e}^{-u^2(z,q)}}{1-\mathrm{Erf}\,u(z,q)}
$$

work out: $$\frac{\partial u}{\partial q} = \frac{1}{\sqrt{2}}\frac{\partial}{\partial q}\frac{\kappa-z\sqrt{q}}{(1-q)^{1/2}} = \ldots = \frac{\kappa\sqrt{q}-z}{2\sqrt{2q}(1-q)^{3/2}}$$

insert into eqn for q:

$$
q\sqrt{q}=\alpha\sqrt{\frac{2}{\pi}}\sqrt{1-q}\int \mathrm{D}z\,\frac{\mathrm{e}^{-u^2(z,q)}(\kappa\sqrt{q}-z)}{1-\mathrm{Erf}\,u(z,q)}
$$

$$2\overline{F} = \log\pi + (1-2\alpha)\log 2 + \frac{1}{1-q} + \log(1-q) + \; 2\alpha\int\mathrm{D}z\;\log\Big[1-\mathrm{Erf}\;u(z,q)\Big]$$

$$q\sqrt{q} = \alpha\sqrt{\frac{2}{\pi}}\sqrt{1-q}\int\mathrm{D}z\;\frac{\mathrm{e}^{-u^2(z,q)}(\kappa\sqrt{q}-z)}{1-\mathrm{Erf}\;u(z,q)}, \qquad u(z,q) = \frac{\kappa-z\sqrt{q}}{\sqrt{2(1-q)}}$$

remember:

$\overline{F}$ =finite: random data linearly separable with margin κ
$\overline{F} = -\infty$: random data not linearly separable with margin κ

- $\alpha = 0$ (so $1 \ll N \ll p$):

  $q = 0, \quad 2\overline{F} = \log\pi + \log 2 + 1$ *random data linearly separable* (*overfitting*)

- $\alpha > 0$ (so $1 \ll N \sim p$):

  transition point: value of α where $q \to 1$

$$1 = \alpha_c(\kappa)\sqrt{\frac{2}{\pi}}\int\mathrm{D}z\;\lim_{q\to 1}\sqrt{1-q}\;\frac{\mathrm{e}^{-[\frac{K-z}{\sqrt{2(1-q)}}]^2}(\kappa-z)}{1-\mathrm{Erf}\Big[\frac{\kappa-z}{\sqrt{2(1-q)}}\Big]}$$

$$\alpha_c(\kappa) = \Big[\frac{1}{\sqrt{\pi}}\int\mathrm{D}z\;(\kappa+z)\lim_{\gamma\to\infty}\frac{1}{\gamma}\,\frac{\mathrm{e}^{-\gamma^2(\kappa+z)^2}}{1-\mathrm{Erf}[\gamma(\kappa+z)]}\Big]^{-1}$$

- remaining limit:

$$\lim_{\gamma\to\infty}\frac{1}{\gamma}\frac{\mathrm{e}^{-\gamma^2 Q^2}}{1-\mathrm{Erf}[\gamma Q]} = Q\sqrt{\pi}\,\theta(Q)$$

proof:

$$Q<0: \qquad \mathrm{Erf}[\gamma Q]\to -1 \quad so \quad \lim_{\gamma\to\infty}\frac{1}{\gamma}\frac{\mathrm{e}^{-\gamma^2 Q^2}}{1-\mathrm{Erf}[\gamma Q]}=0$$

$$Q>0: \qquad \mathrm{Erf}[\gamma Q]=1-\frac{1}{\gamma Q\sqrt{\pi}}\mathrm{e}^{-\gamma^2 Q^2}\Big(1+\mathcal{O}(\frac{1}{\gamma^2 Q^2})\Big)$$

$$\lim_{\gamma\to\infty}\frac{1}{\gamma}\frac{\mathrm{e}^{-\gamma^2 Q^2}}{1-\mathrm{Erf}[\gamma Q]}=\lim_{\gamma\to\infty}\frac{1}{\gamma}\frac{\mathrm{e}^{-\gamma^2 Q^2}}{\frac{1}{\gamma Q\sqrt{\pi}}\mathrm{e}^{-\gamma^2 Q^2}\Big(1+\mathcal{O}(\frac{1}{\gamma^2 Q^2})\Big)}=Q\sqrt{\pi}$$

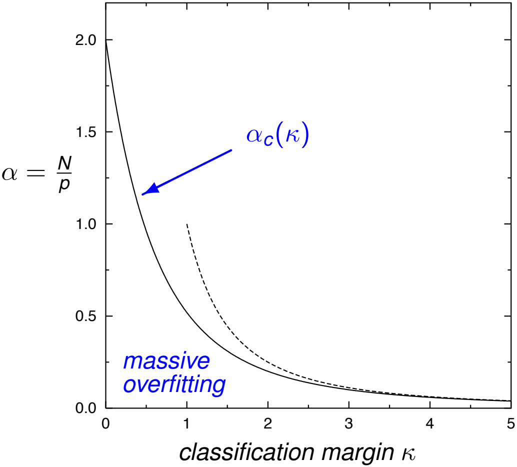
final result

$$\alpha_c(\kappa) = \Big[\int_{-\kappa}^{\infty} \mathrm{D}z\ (\kappa+z)^2\Big]^{-1} \qquad \alpha_c(0) = \Big[\int_0^{\infty} \mathrm{D}z\ z^2\Big]^{-1} = [\tfrac{1}{2}]^{-1} = 2$$

p covariates,
N patients,
binary outcomes,
p and *N* large

<u>random</u> data
(i.e. pure binary noise)
is *perfectly* separable if
$N/p < \alpha_c(\kappa)$

algorithms (SVM etc)
will find pars $\theta_1 \ldots \theta_p$
such that $t_i = sgn[\sum_{\mu=1}^{p} \theta_\mu x_\mu^i]$
for all $i = 1 \ldots N$



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