Modelling of Complex Real-World Systems
Part A. General Methods

A1. Mathematical preliminaries

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Notation and definitions

short-hands and conventions

step function : $\theta(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases}$

sign function : $\mathrm{sgn}(x) = \begin{cases} 1 & \text{for } x > 0 \\ -1 & \text{for } x < 0 \end{cases}$

indicator function : $I[S] = \begin{cases} 1 & \text{if statement } S \text{ is true} \\ 0 & \text{if statement } S \text{ is false} \end{cases}$

Kronecker symbol : $\delta_{ij} = 1 \text{ if } i = j, \quad \delta_{ij} = 0 \text{ if } i \neq j$

complex numbers : $z = a + ib \text{ with } a, b \in \mathrm{I\!R}, \quad \bar{z} = a - ib$

integral boundaries : $\int dx\, f(x) = \int_{-\infty}^{\infty} dx\, f(x)$

averages : $\langle f(x) \rangle = \int dx\, p(x) f(x)$

Hyperbolic functions

$$\cosh(x) = \frac{1}{2}(e^x + e^{-x}), \qquad \sinh(x) = \frac{1}{2}(e^x - e^{-x}), \qquad \tanh(x) = \frac{\sinh(x)}{\cosh(x)}$$

Taylor series

$$\begin{aligned}
e^x &= \sum_{n\geq 0} \frac{x^n}{n!}, \quad \text{for } x \in \mathbb{R} \\
\sin(x) &= \frac{1}{2i}(e^{ix} - e^{-ix}) = \sum_{n\geq 0} (-1)^n \frac{x^{2n+1}}{(2n+1)!}, \quad \text{for } x \in \mathbb{R} \\
\cos(x) &= \frac{1}{2}(e^{ix} + e^{-ix}) = \sum_{n\geq 0} (-1)^n \frac{x^{2n}}{(2n)!}, \quad \text{for } x \in \mathbb{R} \\
(1-x)^{-1} &= \sum_{n\geq 0} x^n, \quad \text{for } |x| < 1 \\
\log(1+x) &= \sum_{n\geq 1} \frac{1}{n}(-1)^{n+1} x^n, \quad \text{for } |x| < 1
\end{aligned}$$

vectors and matrices

vectors in $\mathbb{R}^N$: $\mathbf{x} = (x_1, \ldots, x_N)$

null vector : $\mathbf{0} = (0, \ldots, 0)$

dot product : $\mathbf{x} \cdot \mathbf{y} = \sum_i \bar{x}_i y_i$

orthogonal vectors $\mathbf{x}, \mathbf{y}$: $\mathbf{x} \cdot \mathbf{y} = 0$

$N \times N$ matrices : $\mathbf{A} = \{A_{ij}\}, \quad i, j = 1 \ldots N$

matrix determinant : $\mathrm{Det}(\mathbf{A})$

matrix conjugate $\mathbf{A}^\dagger$: $\mathbf{x} \cdot (\mathbf{A}\mathbf{y}) = (\mathbf{A}^\dagger \mathbf{x}) \cdot \mathbf{y} \;\; \forall (\mathbf{x}, \mathbf{y}), \quad (\mathbf{A}^\dagger)_{ij} = \bar{A}_{ji}$

Hermitian matrix : $\mathbf{A}^\dagger = \mathbf{A}$

symmetric matrix : $A_{ij} = A_{ji}$ *for all* (i, j)

matrix multiplication : $(\mathbf{AB})_{ij} = \sum_k A_{ik} B_{kj}$

identity matrix in $\mathbb{R}^N$: $\mathbb{1}$, with entries $\mathbb{1}_{ij} = \delta_{ij}$

inverse $\mathbf{A}^{-1}$ of $\mathbf{A}$: $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbb{1}$

unitary matrix $\mathbf{U}$: $\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger \mathbf{U} = \mathbb{1}$

Symmetric matrices

symmetric real-valued $N \times N$ matrices $\mathbf{A}$
with entries A_{ij} $(i, j = 1 \ldots N)$

eigenvectors, eigenvalues:

$$\mathbf{Ax} = \lambda \mathbf{x} \quad \text{with} \quad \mathbf{x} \neq \mathbf{0} \qquad \begin{cases} \lambda: & \text{eigenvalue} \\ \mathbf{x}: & \text{eigenvector} \end{cases}$$

general properties

- eigenvalue eqn $\mathrm{Det}(\mathbf{A} - \lambda \mathbb{1}) = 0$ is of order N, hence eigenvalue problem has N solutions λ (which may coincide)
- all eigenvalues λ of $\mathbf{A}$ are real
- all eigenvectors $\mathbf{x}$ of $\mathbf{A}$ can be chosen real-valued
- there exists a complete orthogonal basis in $\mathbb{R}^N$ of eigenvectors: N vectors $\hat{\mathbf{e}}^i = (\hat{e}^i_1, \ldots, \hat{e}^i_N)$, $i=1 \ldots N$, such that

$$\mathbf{A}\hat{\mathbf{e}}^i = \lambda_i \hat{\mathbf{e}}^i \qquad \lambda_i \in \mathbb{R}, \qquad \hat{\mathbf{e}}^i \cdot \hat{\mathbf{e}}^j = \sum_k \hat{e}^i_k \hat{e}^j_k = \delta_{ij}$$

$$\forall \mathbf{x} \in \mathbb{R}^N: \quad \mathbf{x} = \sum_k (\hat{\mathbf{e}}^k \cdot \mathbf{x}) \hat{\mathbf{e}}^k$$

- closure: if $\{\hat{\mathbf{e}}^i\}$ is a normalised orthogonal basis, then $\sum_k \hat{e}_i^k \hat{e}_j^k = \delta_{ij}$

  proof: $$\text{for any } \mathbf{x} \in \mathbb{R}^N: \qquad \sum_j \Big(\sum_k \hat{e}_i^k \hat{e}_j^k \Big) x_j = \sum_k \hat{e}_i^k (\hat{\mathbf{e}}^k \cdot \mathbf{x}) = x_i$$

Diagonalisation of **A**

- construct a new (real-valued) matrix **U** from the components of the normalized eigenvectors $\{\hat{\mathbf{e}}^i\}$, according to $U_{ij} = \hat{e}_i^j$

  claim: **U** is unitary, i.e. $\mathbf{U}^\dagger \mathbf{U} = \mathbf{U}\mathbf{U}^\dagger = \mathbb{1}$

$$\sum_j (\mathbf{U}^\dagger \mathbf{U})_{ij} x_j = \sum_{jk} U_{ki} U_{kj} x_j = \sum_{jk} \hat{e}_k^i \hat{e}_k^j x_j = \sum_j \delta_{ij} x_j = x_i$$

$$\sum_j (\mathbf{U}\mathbf{U}^\dagger)_{ij} x_j = \sum_{jk} U_{ik} U_{jk} x_j = \sum_{jk} \hat{e}_i^k \hat{e}_j^k x_j = \sum_j \delta_{ij} x_j = x_i$$

- **U** brings **A** onto diagonal form:

$$(\mathbf{U}^\dagger \mathbf{A} \mathbf{U})_{ij} = \sum_{kl=1}^N U_{ik}^\dagger A_{kl} U_{lj} = \sum_{kl=1}^N \hat{e}_k^i A_{kl} \hat{e}_l^j = \lambda_j \sum_{k=1}^N \hat{e}_k^i \hat{e}_k^j = \lambda_j \delta_{ij}$$

other properties

- we can always write $A_{ij} = \sum_k \lambda_k \hat{e}_i^k \hat{e}_j^k$
- if all $\lambda_i \neq 0$: inverse $\mathbf{A}^{-1}$ exists, and $(\mathbf{A}^{-1})_{ij} = \sum_k \lambda_k^{-1} \hat{e}_i^k \hat{e}_j^k$
- **A** positive definite symmetric: $\mathbf{x} \cdot \mathbf{A}\mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{R}^N,\ \mathbf{x} \neq \mathbf{0}$
  equivalently: all eigenvalues of **A** have $\lambda_k > 0$
- **A** non-negative definite symmetric: $\mathbf{x} \cdot \mathbf{A}\mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^N,\ \mathbf{x} \neq \mathbf{0}$
  equivalently: all eigenvalues of **A** have $\lambda_k \geq 0$
- any $N \times N$ matrix of the form $A_{ij} = \sum_{\ell=1}^{L} y_{i\ell} y_{j\ell}$, with $y_{i\ell} \in \mathbb{R}$,
  is non-negative definite

  proof:
  $$\mathbf{x} \cdot \mathbf{A}\mathbf{x} = \sum_{ij=1}^{N} x_i A_{ij} x_j = \sum_{\ell=1}^{L} \Big(\sum_{i=1}^{N} x_i y_{i\ell} \Big)^2 \geq 0$$

Gaussian integrals

- one-dimensional:

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

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

- N-dimensional,
  with positive definite **C**:

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

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

general Gaussian distribution
for random variables $\mathbf{x} \in \mathbb{R}^N$

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

with $\boldsymbol{\mu} \in \mathbb{R}^N$,
C positive definite and symmetric

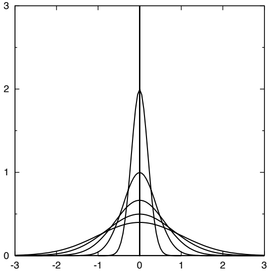
properties

$$\int \mathrm{d}\mathbf{x}\; p(\mathbf{x}) x_i = \mu_i$$

$$\int \mathrm{d}\mathbf{x}\; p(\mathbf{x})(x_i-\mu_i)(x_j-\mu_j) = C_{ij}$$

$$\int \mathrm{d}\mathbf{x}\; p(\mathbf{x}) \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\mu}-\frac{1}{2}\mathbf{k}\cdot\mathbf{C}\mathbf{k}}$$

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

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

  not a function: $\delta(x \neq 0) = 0, \;\; \delta(0) = \infty, \;\; \int \mathrm{d}x \; \delta(x) = 1$

- $\delta(x)$ only has a meaning *inside an integration*, take $\sigma \downarrow 0$ *after* performing the integration

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

  $f(x)$ must be smooth!

- differentiation of $\delta(x)$:

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

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

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 $\delta(x)$: $\delta(x) = \frac{\mathrm{d}}{\mathrm{d}x}\theta(x)$ $\theta(x<0) = 0$, $\theta(x>0) = 1$

proof: both give same result in integrals

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

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

- common expressions for $\delta(x)$:

$$\delta(x) = \lim_{\epsilon\downarrow 0} \frac{\mathrm{e}^{-x^2/2\epsilon^2}}{\epsilon\sqrt{2\pi}}, \qquad \delta(x) = \lim_{\epsilon\downarrow 0} \frac{\epsilon}{\pi}\frac{1}{\epsilon^2+x^2}, \qquad \delta(x) = \lim_{\epsilon\downarrow 0} \frac{\sin(x/\epsilon)}{\pi x}$$

- integral representation:

  use defns of Fourier transforms and their inverse:

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

  apply to $\delta(x)$:

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

- generalization
  to vector arguments: $\mathbf{x} \in \mathbb{R}^N$: $\delta(\mathbf{x}) = \prod_{i=1}^{N} \delta(x_i)$

- probability densities for *functions* of random variables

  $\mathbf{x} \in \mathbb{R}^d$, distributed according to $p(\mathbf{x})$,
  averages $\langle f(\mathbf{x})\rangle = \int \mathrm{d}\mathbf{x}\, p(\mathbf{x}) f(\mathbf{x})$,

  prob distribution of $f(\mathbf{x})$: $p(f) = \langle \delta[f - f(\mathbf{x})]\rangle$

  proof: both give identical averages for all $g(f)$

$$\begin{aligned} \int \mathrm{d}f\, p(f) g(f) &= \int \mathrm{d}f\, g(f) \langle \delta[f - f(\mathbf{x})]\rangle \\ &= \Big\langle \int \mathrm{d}f\, g(f) \delta[f - f(\mathbf{x})] \Big\rangle = \langle g(f(\mathbf{x}))\rangle \end{aligned}$$

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

  proof: both give the same result in integrals

$$\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \left\{ \delta\left[g(x)-g(a)\right] - \frac{\delta(x-a)}{|g'(a)|} \right\} \\
&\quad = \int_{-\infty}^{\infty} \mathrm{d}x\, g'(x) \frac{f(x)}{g'(x)} \delta\left[g(x)-g(a)\right] - \frac{f(a)}{|g'(a)|} \\
&\quad = \int_{g(-\infty)}^{g(\infty)} \mathrm{d}k\, \frac{f(g^{\mathrm{inv}}(k))}{g'(g^{\mathrm{inv}}(k))} \delta\left[k-g(a)\right] - \frac{f(a)}{|g'(a)|} \\
&\quad = \mathrm{sgn}[g'(a)] \frac{f(a)}{g'(a)} - \frac{f(a)}{|g'(a)|} = 0
\end{aligned}$$

more formal definitions and proofs: distribution theory

Steepest descent integration

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

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

- $f(\mathbf{x})$ 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 $\mathbf{x} = \mathbf{x}^\star + \mathbf{y}/\sqrt{N}$:

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

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

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

$$-\lim_{N\to\infty} \frac{1}{N} \log \int_{{\rm I\!R}^p} d\mathbf{x}\; e^{-Nf(\mathbf{x})} = f(\mathbf{x}^\star)$$

proof:

$$\begin{aligned}
&-\lim_{N\to\infty} \frac{1}{N} \log \int_{{\rm I\!R}^p} d\mathbf{x}\; e^{-Nf(\mathbf{x})} \\
&\quad = f(\mathbf{x}^\star) + \lim_{N\to\infty} \Big[\frac{p\log N}{2N} - \frac{1}{N} \log \int_{{\rm I\!R}^p} d\mathbf{y}\; e^{-\frac{1}{2}\sum_{ij} y_i A_{ij} y_j + \mathcal{O}(|\mathbf{y}|^3/\sqrt{N})} \Big] \\
&\quad = f(\mathbf{x}^\star) + \lim_{N\to\infty} \Big[\frac{p\log N}{2N} - \frac{1}{2N} \log \Big(\frac{(2\pi)^p}{\det \mathbf{A}} \Big) - \frac{1}{N} \log \Big(1 + \mathcal{O}\big(\frac{p^{3/2}}{\sqrt{N}}\big) \Big) \Big] \\
&\quad = f(\mathbf{x}^\star) + \lim_{N\to\infty} \Big[\frac{p\log N}{2N} + \mathcal{O}\big(\frac{p}{N}\big) + \mathcal{O}\big(\frac{p^{3/2}}{N^{3/2}}\big) \Big] = f(\mathbf{x}^\star)
\end{aligned}$$

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

- second result, for $p \ll N^{1/3}$:

$$\lim_{N\to\infty} \frac{\int \mathrm{d}\mathbf{x}\; g(\mathbf{x}) \mathrm{e}^{-Nf(\mathbf{x})}}{\int \mathrm{d}\mathbf{x}\; \mathrm{e}^{-Nf(\mathbf{x})}} = g(\mathbf{x}^\star)$$

proof:

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

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

- $f(\mathbf{x})$ 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

  – 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:

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

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

- stuff not mentioned in papers ...

  – in practice we often cannot do the contour deformation in detail
  – multiple extrema? need criteria to pick physical saddle point
  – often we can *choose* the scaling with N of terms in the exponent, what to do? (check Curie-Weiss magnet, very instructive!)

can the requirement $p \ll N/\log N$ be weakened?

more detailed analysis:

$$-\frac{1}{N}\log\int_{\mathbb{R}^p} \mathrm{d}\mathbf{x}\ \mathrm{e}^{-Nf(\mathbf{x})} = f(\mathbf{x}^\star) + \frac{p}{2N}\log(\frac{N}{2\pi}) + \frac{1}{2N}\sum_{i=1}^{p}\log a_i + \frac{p^2}{N^2}\mathcal{O}(S_{1,p}^2) + \frac{p}{N^2}\mathcal{O}(S_{2,p})$$

$$S_{r,p} = \frac{1}{p}\sum_{i=1}^{p} a_i^{-r}, \qquad a_i:\ \text{eigenvalues of } \mathbf{A}$$

e.g. if $S_{r,p} = \mathcal{O}(1)$:
can use steepest descent for $p \ll N$

Exponential distributions

stochastic processes for *microscopic* $\mathbf{x}\in X\subseteq \mathbb{R}^N$, often with large N,
that evolve to a stationary state, with prob distribution $p(\mathbf{x})$
many of the *exponential* form ...

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

$$\sum_{\mathbf{x}\in X} p(\mathbf{x})\omega_1(\mathbf{x}) = \Omega_1, \;\ldots\;, \sum_{\mathbf{x}\in X} p(\mathbf{x})\omega_L(\mathbf{x}) = \Omega_L, \qquad (\Omega_1,\ldots,\Omega_L): \text{ macroscopic description with } L \ll N$$

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

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

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

$$\text{subject to} \quad \begin{cases} p(\mathbf{x}) \geq 0 \;\; \forall \mathbf{x}, \;\; \sum_{\mathbf{x}\in X} p(\mathbf{x}) = 1 \\ \sum_{\mathbf{x}\in X} p(\mathbf{x})\omega_\ell(\mathbf{x}) = \Omega_\ell \;\; \text{for all } \ell = 1\ldots L \end{cases}$$

- solution using Lagrange's method:

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

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

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

- 'exponential distribution':

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

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

example: physical systems in 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

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

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

- define

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

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

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

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