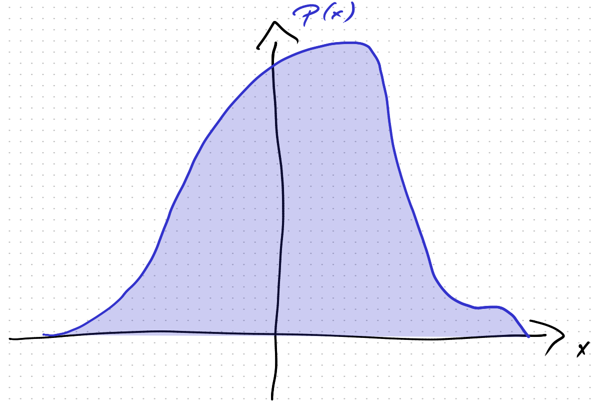
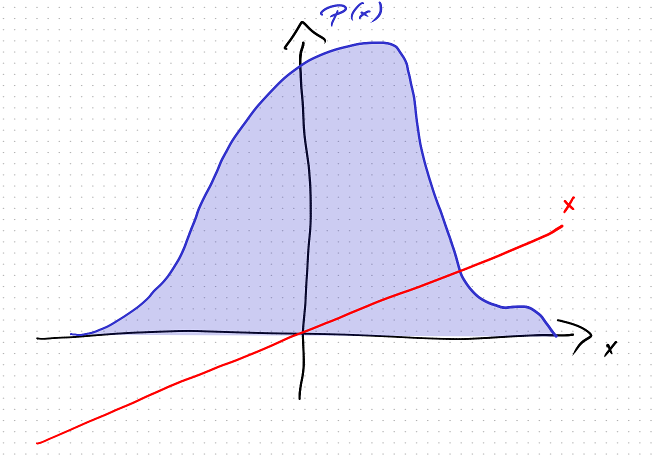
4.8 Maximum Entropy with known 1st and 2nd Moments



4.8 Maximum Entropy with known 1st and 2nd Moments



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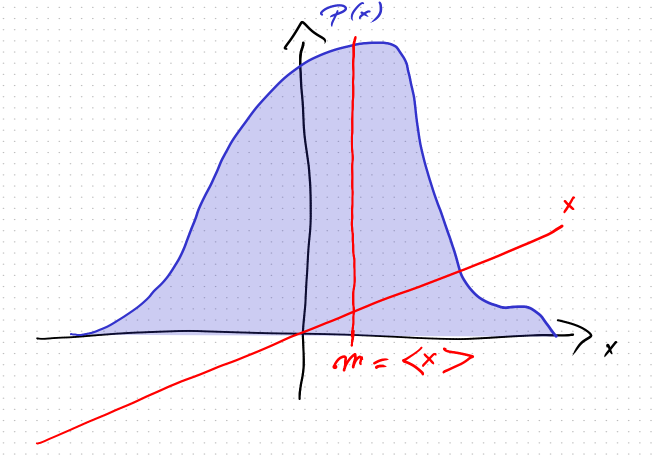

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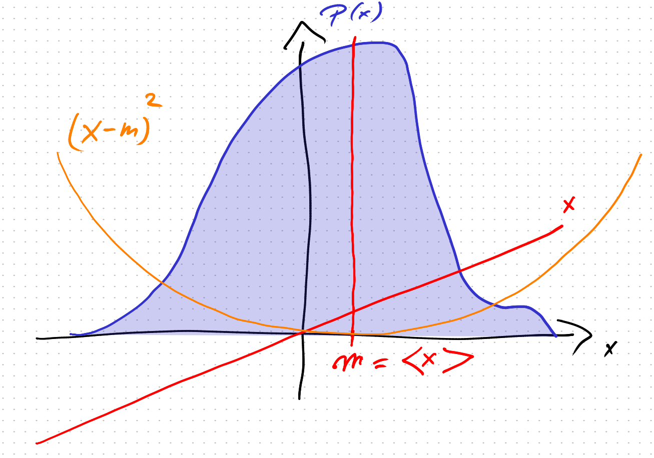

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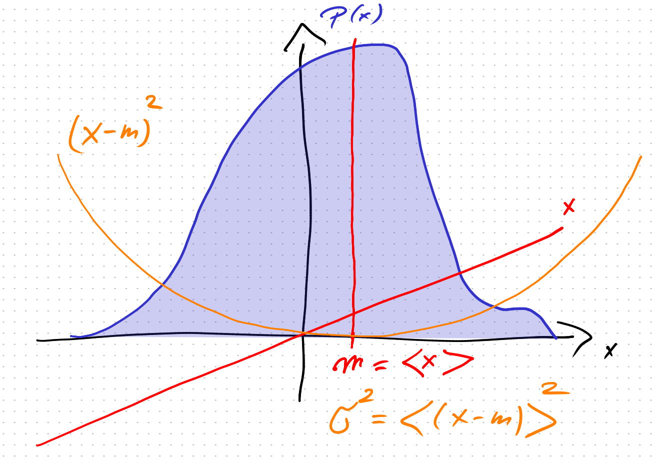

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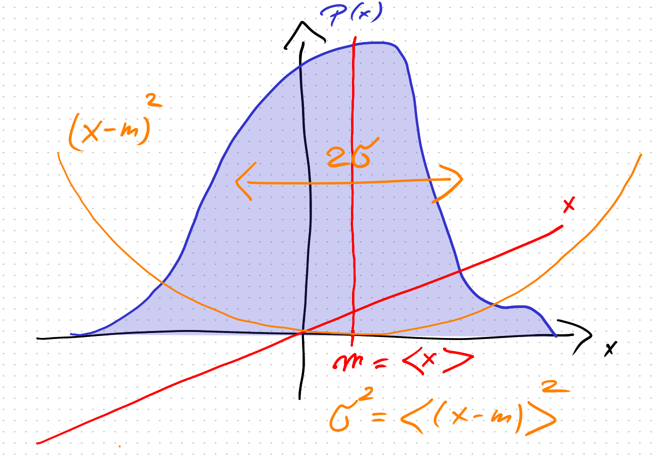

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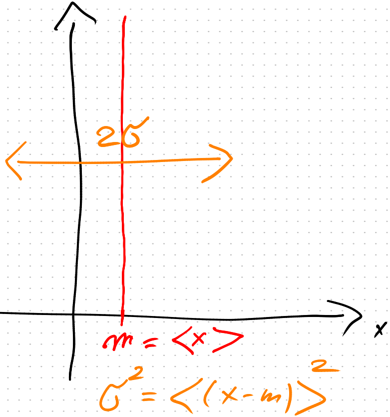

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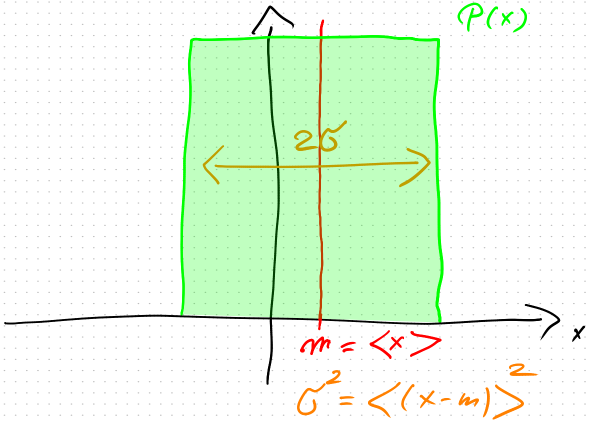

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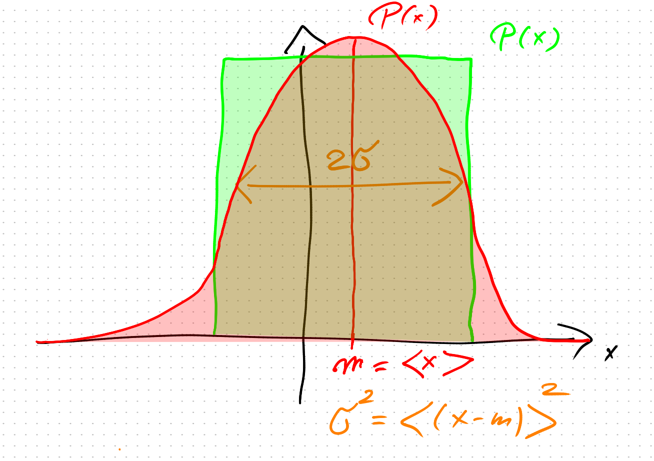

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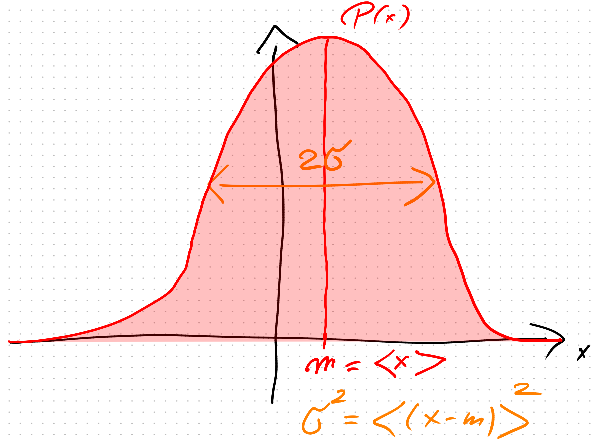


4.8 Maximum Entropy with known 1^{st} and 2^{nd} Moments

Prior information I: $x \in \mathbb{R}$
Prior knowledge: $q(x) := \mathcal{P}(x|I) = \text{const.}$
Updating information J: $\langle x \rangle_{(x|J,I)} = m$, $\langle (x-m)^2 \rangle_{(x|J,I)} = \sigma^2$
Posterior knowledge: $p(x) := \mathcal{P}(x|J,\,I) = \frac{e^{\alpha x + \beta (x-m)^2}}{\mathcal{Z}(\alpha,\,\beta)}$
1. calculate $\mathcal{Z}(\alpha,\,\beta)$:

$$
\begin{aligned}
\mathcal{Z}(\alpha,\,\beta) &= \int_{-\infty}^{\infty} dx\, e^{\alpha x + \beta (\underbrace{x-m}_{=x'})^2} \\
&= \int_{-\infty}^{\infty} dx'\, e^{\alpha x' + \alpha m + \beta x'^2}
\end{aligned}
$$

4.8 Maximum Entropy with known 1st and 2nd Moments

$$\mathcal{Z}(\alpha,\,\beta) = \int_{-\infty}^{\infty} dx'\, e^{\alpha x' + \alpha m + \beta x'^2}$$

Completing the square:
$$= e^{\alpha m} \int_{-\infty}^{\infty} dx'\, e^{\beta\left(x'^2 + \frac{2\alpha x'}{2\beta} + \frac{\alpha^2}{(2\beta)^2}\right) - \frac{\alpha^2}{4\beta}}$$

$$= e^{\alpha m - \frac{\alpha^2}{4\beta}} \int_{-\infty}^{\infty} dx'\, e^{\beta\left(x' + \frac{\alpha}{2\beta}\right)^2}$$

Claiming $\beta < 0$:
$$= e^{\alpha m + \frac{\alpha^2}{4\,|\beta|}} \int_{-\infty}^{\infty} dx'\, e^{-|\beta|\,\left(x' - \frac{\alpha}{2|\beta|}\right)^2}$$

$$= e^{\alpha m + \frac{\alpha^2}{4\,|\beta|}} \sqrt{\frac{\pi}{-\beta}}$$

4.8 Maximum Entropy with known 1st and 2nd Moments

2. determine α and β:

$$
\begin{aligned}
\ln \mathcal{Z}(\alpha,\, \beta) &= \alpha m - \frac{\alpha^2}{4\beta} + \frac{1}{2}\ln\left(\frac{\pi}{-\beta}\right) \\
\frac{\partial \ln \mathcal{Z}(\alpha,\, \beta)}{\partial \alpha} &= m - \frac{\alpha}{2\beta} \stackrel{!}{=} m \\
\Rightarrow \alpha &= 0 \\
\frac{\partial \ln \mathcal{Z}(\alpha = 0,\, \beta)}{\partial \beta} &= -\frac{1}{2\beta} \stackrel{!}{=} \sigma^2 \\
\Rightarrow \beta &= -\frac{1}{2\sigma^2}
\end{aligned}
$$

Insert in $\mathcal{Z}(\alpha,\, \beta)$:

$$
\mathcal{Z} = \sqrt{2\pi\sigma^2}
$$

4.8 Maximum Entropy with known 1st and 2nd Moments

3. calculate $p(x) = \mathcal{P}(x|J, I)$**:**

$$
\begin{aligned}
P(x|J, I) &= \left.\frac{e^{\alpha x+\beta(x-m)^2}}{\mathcal{Z}(\alpha, \beta)}\right|_{\alpha=0,\beta=-1/(2\sigma^2)} \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-m)^2}{2\sigma^2}} \\
&= \mathcal{G}(x-m, \sigma^2)
\end{aligned}
$$

$\Rightarrow$ Maximum Entropy PDF $P(x|J, I)$ for known 1st and 2nd moments (and flat prior) is Gaussian distribution

5 Gaussian Distribution

- maximum Entropy solution if only 1^{st} and 2^{nd} moments known
- emerges according to central limit theorem
- mathematically convenient

5.1 One dimensional Gaussian distribution:

$$\mathcal{G}(x-m,\,\sigma_x^2) \quad = \quad \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp\left(-\frac{(x-m)^2}{2\,\sigma_x^2}\right)$$

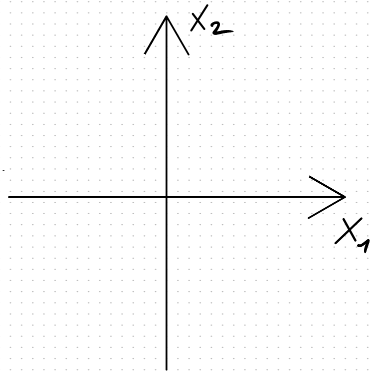
5.2 Multivariate Gaussian Distribution

$x = (x_1, \dots x_n)^{\mathrm{t}}$: zero centered independent Gaussian distributed variables
$\sigma_1^2, \dots \sigma_n^2$: corresponding variances
$X = \mathrm{diag}(\sigma_1^2, \dots \sigma_n^2)$: diagonal covariance matrix

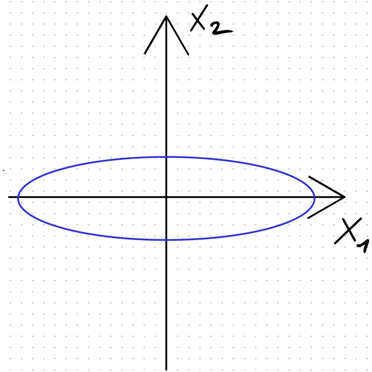
$$\begin{aligned}
\text{Joint probability: } \mathcal{P}(x) &= \prod_{i=1}^{n} \mathcal{P}(x_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{(x_i)^2}{2\,\sigma_i^2}\right) \\
&= \frac{1}{\prod_{i=1}^{n} \sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{1}{2}\sum_{i=1}^{n} \frac{x_i^2}{\sigma_i^2}\right) = \frac{1}{\sqrt{|2\pi X|}} \exp\left(-\frac{1}{2} x^{\dagger} X^{-1} x\right)
\end{aligned}$$

$$\text{Multivariate Gaussian: } \mathcal{G}(x,\, X) = \frac{1}{\sqrt{|2\pi X|}} \exp\left(-\frac{1}{2} x^{\dagger} X^{-1} x\right)$$

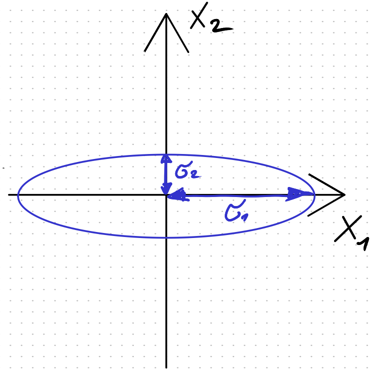
Orthonormal transformation



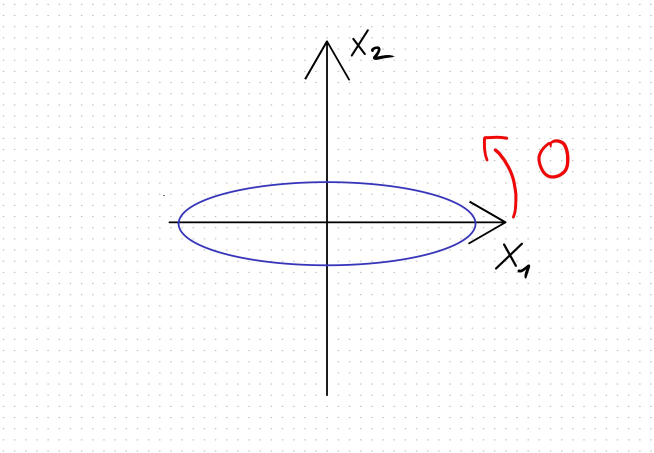
Orthonormal transformation



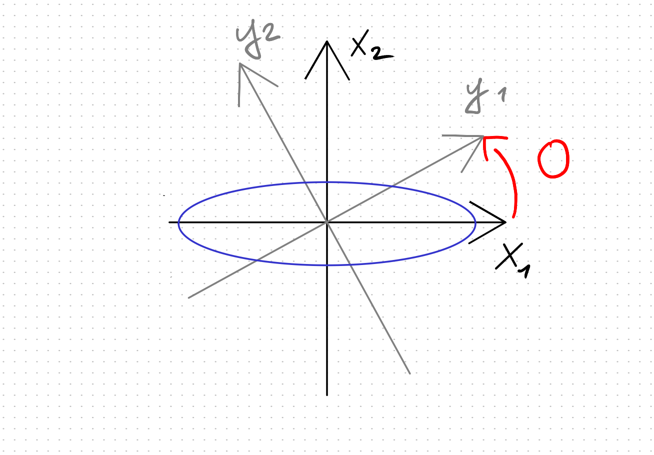
Orthonormal transformation



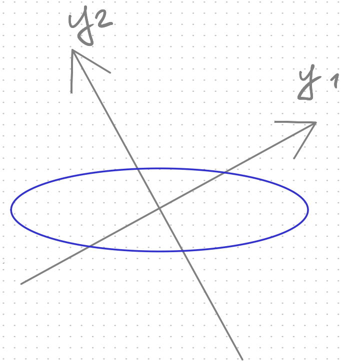
Orthonormal transformation



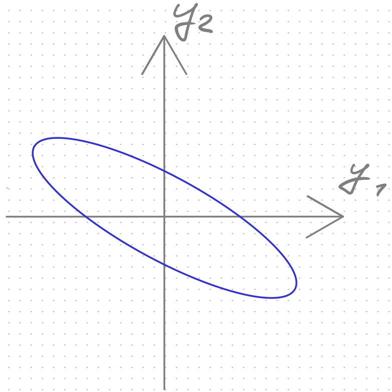
Orthonormal transformation



Orthonormal transformation



Orthonormal transformation



From independent to dependent coordinates

Orthonormal basis transformation in n-dim. space:

$$\begin{aligned} y &= O\,x \\ O^{-1} &= O^{\dagger} \end{aligned}$$

$$\begin{aligned} &\Rightarrow \quad |O| = |O^{\dagger}| = |O^{-1}| = 1/|O| \\ &\Rightarrow \quad |O|^2 = 1 \\ &\Rightarrow \quad \|O\| = \|O^{\dagger}\| = 1 \end{aligned}$$

Conservation of probability mass:

$$\mathcal{P}(y|I)\,dy \quad = \quad \mathcal{P}(x|I)\,dx\big|_{x=O^{\dagger}y}$$

From independent to dependent coordinates

$$
\begin{aligned}
\Rightarrow \mathcal{P}(y|I) &= \mathcal{G}(x, X) \left\| \frac{\partial x}{\partial y} \right\| \Bigg|_{x=O^\dagger y} = \mathcal{G}(O^\dagger y, X) \underbrace{\|O^\dagger\|}_{=1} \\
&= \frac{1}{\sqrt{|2\pi X|}} \exp\left(-\frac{1}{2} \underbrace{(O^\dagger y)^\dagger}_{x^\dagger = y^\dagger O} X^{-1} \underbrace{O^\dagger y}_{x} \right) \\
&= \frac{1}{\sqrt{|2\pi X|}} \exp\left(-\frac{1}{2} y^\dagger \underbrace{O X^{-1} O^\dagger}_{Y^{-1}} y \right) \\
&= \frac{1}{\sqrt{|2\pi X|}} \exp\left(-\frac{1}{2} y^\dagger Y^{-1} y \right)
\end{aligned}
$$

From independent to dependent coordinates

$$
\begin{aligned}
|Y| &= |Y^{-1}|^{-1} \\
&= |OX^{-1}O^{\dagger}|^{-1} \\
&= (\underbrace{|O|}_{=\pm 1}\,|X^{-1}|\,\underbrace{|O^{\dagger}|}_{=\pm 1})^{-1} \\
&= |X|
\end{aligned}
$$

Generic multivariate Gaussian:

$$\Rightarrow \mathcal{P}(y) = \mathcal{G}(y,\, Y) = \frac{1}{\sqrt{|2\pi Y|}} \exp\left(-\frac{1}{2} y^{\dagger} Y^{-1} y\right)$$

Moments of the multivariate Gaussian

Normalization:

$$
\begin{aligned}
\langle 1 \rangle_{\mathcal{G}(y,\,Y)} &= \int dy\, 1\, \mathcal{G}(y,\, Y) = \int dx\, 1\, \mathcal{G}(x,\, X) = 1 \\
1 &= \frac{1}{\sqrt{|2\pi Y|}} \underbrace{\int dy \,\exp\left(-\frac{1}{2} y^\dagger Y^{-1} y\right)}_{=\sqrt{|2\pi Y|}}
\end{aligned}
$$

1^{st} Moment:

$$
\begin{aligned}
\langle y \rangle_{\mathcal{G}(y,\,Y)} &= \int dy\, y\, \mathcal{G}(y,\, Y) \\
&= \int dy' \,(-y')\, \mathcal{G}(-y',\, Y) \| -\mathbb{1} \| \\
&= -\langle y' \rangle_{\mathcal{G}(y',\,Y)} = 0
\end{aligned}
$$

Moments of the multivariate Gaussian

2nd Moment:

$$\left\langle y\, y^\dagger \right\rangle_{\mathcal{G}(y,Y)} = \int dy\, y\, y^\dagger \mathcal{G}(y,\, Y)$$

$$= \int dx\, \mathcal{G}(x,\, X) O x x^\dagger O^\dagger$$

$$= O \int dx\, x\, x^\dagger \mathcal{G}(x,\, X)\, O^\dagger \stackrel{?}{=} O X O^\dagger = Y$$

$$\int dx\, x_i\, x_j\, \mathcal{G}(x,\, X) = \left[\prod_{k=1}^{n} \int dx_k \mathcal{G}(x_k, \sigma_k^2) \right] x_i\, x_j$$

$$= \begin{cases} \left[\int dx_i \mathcal{G}(x_i, \sigma_i^2)\, x_i \right] \left[\int dx_j \mathcal{G}(x_j, \sigma_j^2)\, x_j \right] & \text{if } i \neq j \\ \int dx_i \mathcal{G}(x_i, \sigma_i^2)\, x_i^2 & \text{if } i = j \end{cases}$$

$$= \begin{cases} 0 & \text{if } i \neq j \\ \sigma_i^2 & \text{if } i = j \end{cases} = \delta_{ij} \sigma_i^2 = X_{ij} \;\square$$

Moments of the multivariate Gaussian

$$\begin{aligned}
\langle y \rangle_{\mathcal{G}(y,\,Y)} &= 0 \\
\langle f(y) \rangle_{\mathcal{G}(y,\,Y)} &= 0, \ \text{if} \, f(-y) = -f(y) \\
\langle y y^{\dagger} \rangle_{\mathcal{G}(y,\,Y)} &= Y
\end{aligned}$$

Wick theorem

Wick theorem:

$\mathbb{P}$: set of all possible ways to partition $\{i_1, \ldots, i_{2n}\}$ into pairs

$$\langle y_{i_1} \ldots y_{i_{2n}} \rangle_{\mathcal{G}(y,\,Y)} = \langle \prod_{j=1}^{2n} y_{i_j} \rangle_{\mathcal{G}(y,\,Y)} = \sum_{p \in \mathbb{P}} \prod_{(i',j') \in p} Y_{i_{i'} i_{j'}}$$

Examples:

- $\langle y_{i_1} y_{i_2} \rangle_{\mathcal{G}(y,\,Y)} = Y_{i_1 i_2}$
- $\langle y_{i_1} y_{i_2} y_{i_3} y_{i_4} \rangle_{\mathcal{G}(y,\,Y)} = Y_{i_1 i_2} Y_{i_3 i_4} + Y_{i_1 i_3} Y_{i_2 i_4} + Y_{i_1 i_4} Y_{i_2 i_3}$

$$\Rightarrow \quad \langle y_i^{2n} \rangle_{\mathcal{G}(y,\,Y)} = \frac{(2n)!}{2^n n!} (Y_{ii})^n$$

$$\Rightarrow \quad \langle y_i^{2n+1} \rangle_{\mathcal{G}(y,\,Y)} = 0$$

Maximum Entropy with known n-dimensional 1st and 2nd Moments

Prior information I: $s \in V$ (e.g. $\mathbb{R}$, $\mathbb{R}^n$, $C(\mathbb{R}^n)$)
Prior knowledge: $q(s) := \mathcal{P}(s|I) = \text{const.} = 1$
Updating information J: $\langle s \rangle_{(s|J,I)} = m$, $\langle (s-m)(s-m)^\dagger \rangle_{(s|J,I)} = S$
Posterior: $p(s) = \frac{1}{\mathcal{Z}} \exp[\sum_i \mu_i (s-m)_i + \sum_{ij} \Lambda_{ij} \underbrace{((s-m)_i(s-m)_j - S_{ji})}_{=B_{ji}(s)}]$

1. calculate $\mathcal{Z}(\mu, \Lambda)$:

$$
\begin{aligned}
\mathcal{Z}(\mu, \Lambda) &= \int ds \exp\left[\mu^\dagger \underbrace{(s-m)}_{s'} + \text{Tr}[\Lambda B(s)]\right] \\
&= \int ds' \exp\left[\mu^\dagger s' + \text{Tr}[\Lambda(s' s'^\dagger - S)]\right] \\
&= \int ds' \exp\left[\mu^\dagger s' + s'^\dagger \Lambda s' - \text{Tr}[\Lambda S]\right] = e^{-\text{Tr}[\Lambda S]} \int ds' \, e^{\mu^\dagger s' + s'^\dagger \Lambda s'}
\end{aligned}
$$

Maximum Entropy with known n-dimensional 1st and 2nd Moments

2. determine μ and Λ:

$$\ln \mathcal{Z}(\mu,\, \Lambda) = -\mathrm{Tr}[\Lambda S] + \ln\left(\int ds' \, \exp(\mu^\dagger s' + s'^\dagger \Lambda s')\right)$$

$$\frac{\partial \ln \mathcal{Z}(\mu,\, \Lambda)}{\partial \mu} = \left(\frac{\partial \ln \mathcal{Z}}{\partial \mu_i}\right)_i = \frac{\int ds' \, s' \exp(\mu^\dagger s' + s'^\dagger \Lambda s')}{\int ds' \, \exp(\mu^\dagger s' + s'^\dagger \Lambda s')} \stackrel{!}{=} 0$$

$$\Rightarrow \mu = 0$$

$$\frac{\partial \ln \mathcal{Z}(\mu,\, \Lambda)}{\partial \Lambda} = \left(\frac{\partial \ln \mathcal{Z}}{\partial \Lambda_{ij}}\right)_{ij} = \underbrace{-(S_{ji})_{ij}}_{=-S} + \left(\frac{\int ds' \, s'_i s'_j \exp(s'^\dagger \Lambda s')}{\int ds' \, \exp(s'^\dagger \Lambda s')}\right)_{ij} \stackrel{!}{=} 0$$

$$\Rightarrow S = \frac{\int ds' \, s' s'^\dagger \exp\left(-\frac{1}{2} s'^\dagger (-\frac{1}{2}\Lambda^{-1})^{-1} s'\right)}{\int ds' \exp\left(-\frac{1}{2} s'^\dagger (-\frac{1}{2}\Lambda^{-1})^{-1} s'\right)} = \frac{\int ds' \, s' s'^\dagger \mathcal{G}\left(s', -\frac{1}{2}\Lambda^{-1}\right)}{\int ds' \mathcal{G}\left(s', -\frac{1}{2}\Lambda^{-1}\right)}$$

$$= -\frac{1}{2}\Lambda^{-1} \Rightarrow \Lambda = -\frac{1}{2} S^{-1}$$

Maximum Entropy with known n-dimensional 1st and 2nd Moments

Insert in $\mathcal{Z}(\mu, \Lambda)$:

$$\begin{aligned}\mathcal{Z}(\mu, \Lambda) &= \int ds' \exp\left[-\frac{1}{2} s'^{\dagger} S^{-1} s' + \frac{1}{2} \mathrm{Tr}[\underbrace{S^{-1} S}_{=\mathbb{1}}] \right] \\ &= |2\pi S|^{1/2} e^{\frac{1}{2}\mathrm{Tr}[\mathbb{1}]}\end{aligned}$$

3. calculate $p(s) = \mathcal{P}(s|J, I)$**:** remember: $s' = s - m$

$$\begin{aligned}P(s|J, I) &= \frac{1}{\sqrt{|2\pi S|}} \exp\left(-\frac{1}{2} (s-m)^{\dagger} S^{-1} (s-m) \right) \\ &= \mathcal{G}(s-m, S)\end{aligned}$$

⇒use Gaussian distribution $\mathcal{G}(s-m, S)$ given the n-dim. mean m and variance S