Pattern Recognition

Review of Prerequisites in Math and Statistics

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Based on
Appendix chapters of
Pattern Recognition, 4th Ed.
by S. Theodoridis and K. Koutroumbas
and figures from
Wikipedia.org

Probability and Statistics

- **Probability** P(*A*) of an event *A* : a real number between 0 to 1.
- **Joint probability** P(A ∩ B) : probability that both A and B occurs in a single experiment.

  P(A ∩ B) = P(A)P(B) if A and B and **independent**.
- Probability P(A ∪ B) of union of A and B: either A or B occurs in a single experiment.

  P(A ∪ B) = P(A) + P(B) if A and B are mutually exclusive.

- **Conditional probability**:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}$$

- Therefore, the **Bayes rule**:

$$P(A|B)P(B) = P(B|A)P(A) \text{ and } P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

- **Total probability:** let $A_1, \ldots, A_m$ such that $\sum_{i=1}^{m} P(A_i) = 1$ then

$$P(B) = \sum_{i=1}^{m} P(B|A_i)P(A_i)$$

- **Probability density function (pdf)**: p(x) for a continuous random variable x

$$P(a \le x \le b) = \int_a^b p(x)dx$$

Total and conditional probabilities can also be extended to pdf's.

- **Mean** and **Variance**: let p(x) be the pdf of a random variable x

$$E[x] = \int_{-\infty}^{+\infty} xp(x)dx, \text{ and } \sigma^2 = \int_{-\infty}^{+\infty} (x - E[x])^2 p(x)dx$$

- **Statistical independence**:

$$p(x, y) = p_x(x)p_y(y)$$

- **Kullback-Leibler divergence (Distance?) of pdf's**

$$L(p(\mathbf{x}), p'(\mathbf{x})) = -\int p(\mathbf{x}) \ln \frac{p'(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}$$

Pay attention that $L(p(\mathbf{x}), p'(\mathbf{x})) \ne L(p'(\mathbf{x}), p(\mathbf{x}))$

- **Characteristic function** of a pdf:

$$\Phi(\mathbf{\Omega}) = \int_{-\infty}^{+\infty} p(\mathbf{x}) \exp(j\mathbf{\Omega}^T \mathbf{x}) d\mathbf{x} = E[\exp(j\mathbf{\Omega}^T \mathbf{x})]$$

$$\Phi(s) = \int_{-\infty}^{+\infty} p(x) \exp(sx) dx = E[\exp(sx)]$$

- **2nd Characteristic function:** $\Psi(s) = \ln \Phi(s)$

- **n-th order moment**: $\dfrac{d^n \Phi(0)}{ds^n} = E[x^n]$

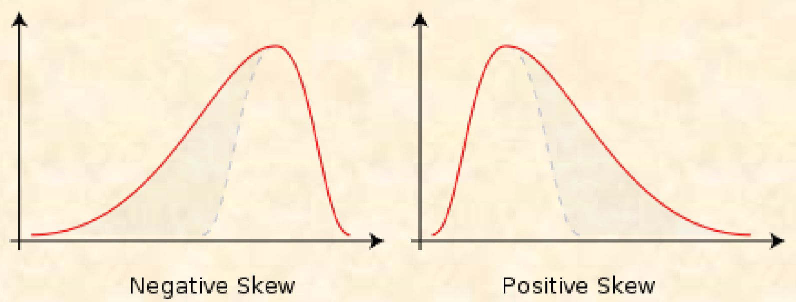
- **Cumulants**: $\kappa_n = \dfrac{d^n \Psi(0)}{ds^n}$

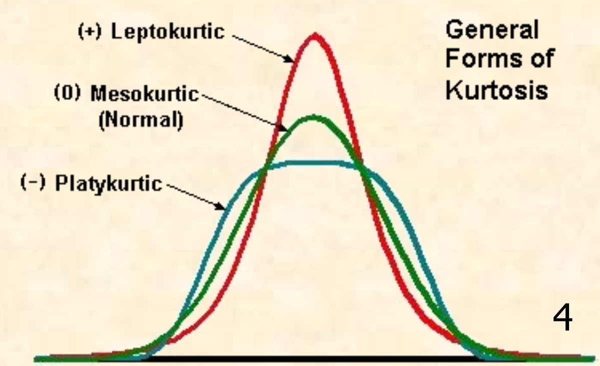
When $E[x] = 0$, then

$\kappa_0 = 0, \kappa_1 = E[x] = 0,$

$\kappa_2 = E[x^2] = \sigma^2, \kappa_3 = E[x^3]$ (Skewness)

$\kappa_4 = E[x^4] - 3\sigma^4$ (Kurtosis)





Discrete Distributions

- **Binomial distribution B(n,p):**

  Repeatedly grab n balls, each with a probability p of getting a black ball. The probability of getting k black balls:

$$P(k) = \binom{n}{k} p^k (1-p)^{n-k}$$

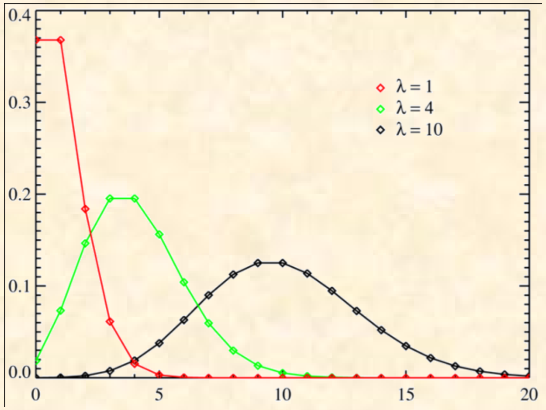
- **Poisson distribution**

  probability of # of events occurring in a fixed period of time if these events occur with a known average.

$$P(k;\lambda) = \frac{\lambda^k e^{-\lambda}}{k!}$$

When $n \to \infty$ and np remains constant,

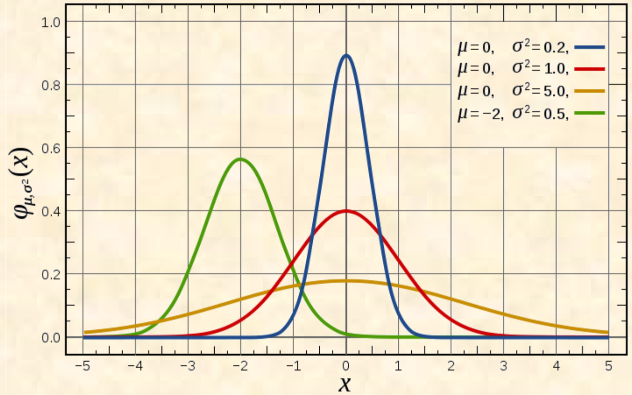
$B(n, p) \to Poisson(np)$



Normal (Gaussian) Distribution

- **Univariate N(μ, σ²):**

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{(x-\mu)^2}{2\sigma^2})$$



- **Multivariate N(μ, Σ):**

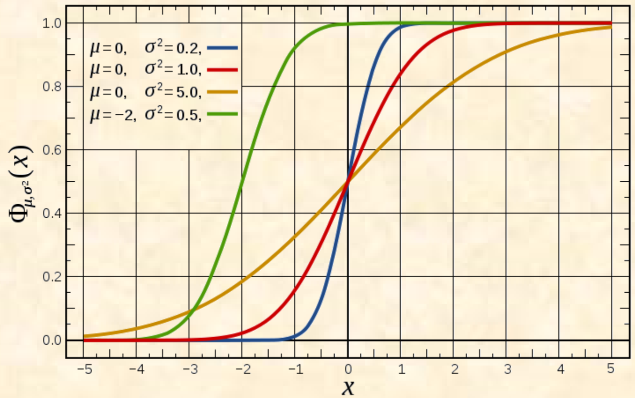
$$p(x) = \frac{1}{\sqrt{2\pi|\Sigma|}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$$

with the mean μ and the covariance matrix

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1l} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2l} \\ \vdots & \vdots & \vdots & \vdots \\ \sigma_{l1} & \sigma_{l2} & \cdots & \sigma_l^2 \end{bmatrix}$$

where $\sigma_i^2 = E[(x_i - \mu_i)^2]$ and

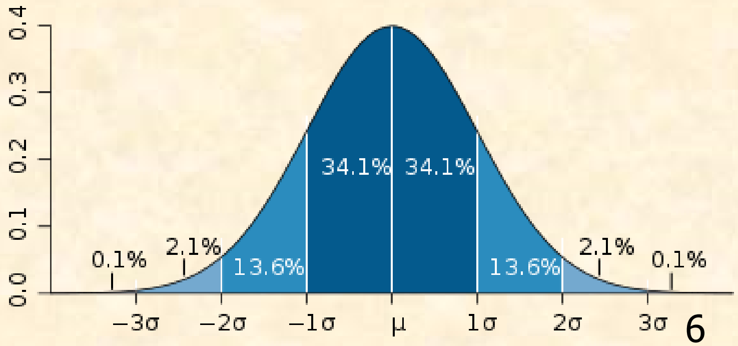
$\sigma_{ij} = \sigma_{ji} = E[(x_i - \mu_i)(x_j - \mu_j)]$



- **Central limit theorem:**

Let $z = \sum_{i=1}^{n} x_i$, then $\frac{z-\mu}{\sigma} \sim N(0,1)$ when $n \to \infty$

irrespective of the pdf's of x_i's.



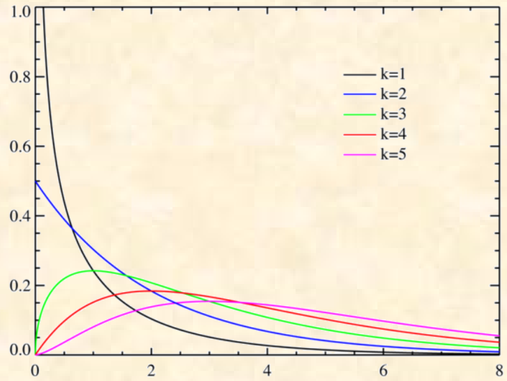
Other Continuous Distributions

- **Chi-square (X^2) distribution** of k degrees of freedom:

  distribution of a sum of squares of *k* independent standard normal random variables, that is, $\chi^2 = x_1^2 + x_2^2 + \cdots + x_k^2$ where $x_i \approx N(0,1)$

$$p(y) = \frac{1}{2^{k/2}\Gamma(k/2)} y^{k/2-1} e^{-y/2} \text{step}(y),$$

$$\text{where } \Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt$$



- Mean: k, Variance: 2k

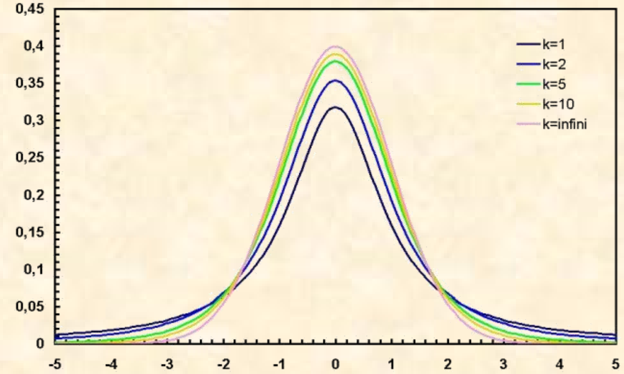
- Assume $x \sim \chi^2(k)$
  - Then $(x-k)/\sqrt{2k} \sim N(0,1)$ as $k \to \infty$ by central limit theorem.
  - Also $\sqrt{2x}$ is approximately normally distributed with mean $\sqrt{2k-1}$ and **unit variance.**

Other Continuous Distributions

- **t-distribution:** estimating mean of a normal distribution when sample size is small.

  A t-distributed variable $q = x/\sqrt{z/k}$ where $x \approx N(0,1)$ and $z \approx \chi^2(k)$

$$p(q) = \frac{\Gamma((k+1)/2)}{\sqrt{\pi k}\,\Gamma(k/2)}\left(1+\frac{q^2}{k}\right)^{-(k+1)/2}$$



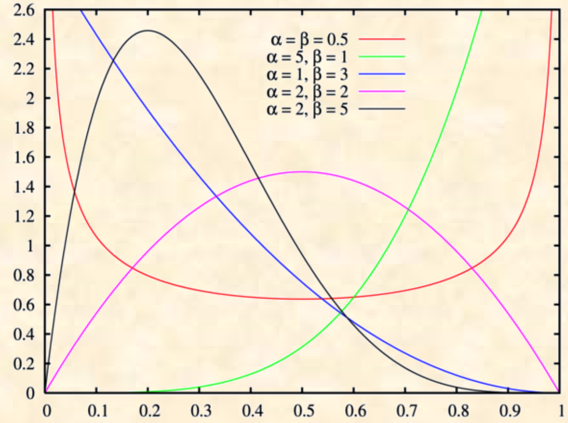
  Mean: 0 for k > 1,

  variance: k/(k-2) for k > 2

- **β-distribution:** Beta(α,β): the posterior distribution of *p* of a binomial distribution after α−1 events with *p* and β − 1 with 1 − *p*.

$$p(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

$$= \frac{1}{\mathrm{B}(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$



Linear Algebra

- Eigenvalues and eigenvectors:

  there exists λ and v such that $Av = \lambda v$
- Real matrix A is called *positive semidefinite* if $x^T A x \geq 0$ for **every** nonzero vector x;

  A is called *positive definite* if $x^T A x > 0$.
- Positive definite matrixes act as positive numbers.

  All positive eigenvalues
- If A is symmetric, $A^T = A$,

  then its eigenvectors are orthogonal, $v_i^T v_j = 0$.
- Therefore, a symmetric A can be diagonalized as

$$A = \Phi \Lambda \Phi^T \text{ and } \Phi^T A \Phi = \Lambda$$

$$\text{where } \Phi = [v_1, v_2, \ldots v_l] \text{ and } \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots \lambda_l)$$

Correlation Matrix and Inner Product Matrix

Principal component analysis (PCA)

- Let x be a random variable in R^l, its correlation matrix $\Sigma=E[xx^T]$ is positive semidefinite and thus can be diagonalized as

$$\Sigma = \Phi \Lambda \Phi^T$$

- Assign $x' = \Phi^T x$, then $\Sigma' = E(x' x'^T) = \Phi^T \Sigma \Phi = \Lambda$
- Further assign $x'' = \Lambda^{-1/2} \Phi^T x$, then $\Sigma'' = E(x'' x''^T) = I$

Classical multidimensional scaling (classical MDS)

- Given a distance matrix $D=\{d_{ij}\}$, the inner product matrix $G=\{x_i^T x_j\}$ can be computed by a bidirectional centering process

$$G = -\frac{1}{2}(I - \frac{1}{n} ee^T) D (I - \frac{1}{n} ee^T) \text{ where } e = [1,1,\ldots,1]^T$$

- G can be diagnolized as $G = \Psi \Lambda' \Psi^T$
- Actually, $n\Lambda$ and Λ' share the same set of eigenvalues, and

$$\Phi = X^T \Psi \text{ where } X = [x_1,\ldots,x_n]^T$$

$$\text{Because } G = XX^T, X \text{ can then be receovered as } X = \Psi \Lambda'^{1/2}$$

Cost Function Optimization

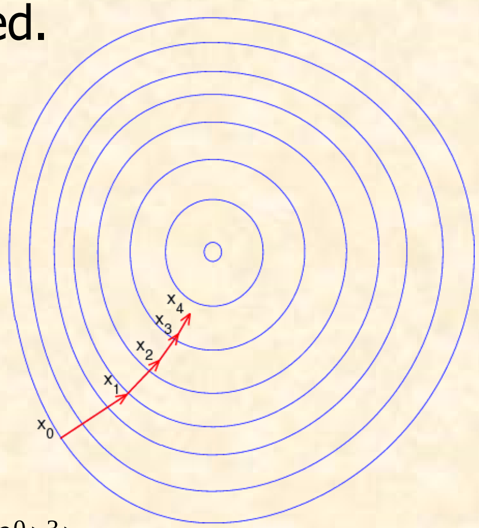
❖ Find θ so that a differentiable function J(θ) is minimized.

❖ **Gradient descent method**

- Starts with an initial estimate θ(0)
- Adjust θ iteratively by

$$\theta_{new} = \theta_{old} + \Delta\theta$$

$$\Delta\theta = -\mu \frac{\partial J(\theta)}{\partial \theta}\Big|_{\theta=\theta_{old}}, \text{ where } \mu > 0$$



- Taylor expansion of J(θ) at a stationary point θ^0

$$J(\theta) = J(\theta^0) + (\theta-\theta^0)^T \mathbf{g} + \frac{1}{2}(\theta-\theta^0)^T \mathbf{H}(\theta-\theta^0) + O((\theta-\theta^0)^3)$$

$$\text{where } \mathbf{g} = \frac{\partial J(\theta)}{\partial \theta}\Big|_{\theta=\theta^0} \text{ and } \mathbf{H}(i,j) = \frac{\partial^2 J(\theta)}{\partial\theta_i \partial\theta_j}\Big|_{\theta=\theta^0}$$

Ignore higher order terms within a neighborhood of θ^0

$$\theta_{new} - \theta^0 = (I - \mu\mathbf{H})(\theta_{old} - \theta^0)$$

$\mathbf{H}$ is positive semidefinite, then $\mathbf{H} = \Phi\Lambda\Phi^T$, we get

$$\Phi^T(\theta_{new} - \theta^0) = (I - \mu\Lambda)\Phi^T(\theta_{old} - \theta^0)$$

which will converge if every $|1-\mu\lambda_i| < 1$, i.e., $\mu < 2/\lambda_{\max}$.

Therefore, the convergence speed is decided by $\lambda_{\min}/\lambda_{\max}$.

❖ Newton's method

- Adjust θ iteratively by

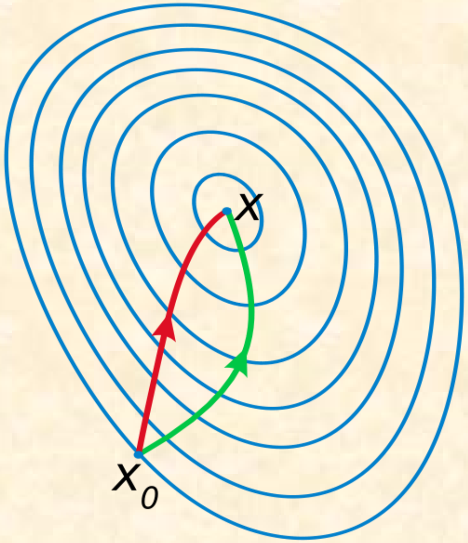
$$\Delta\theta = -\mathbf{H}_{old}^{-1}\frac{\partial J(\theta)}{\partial\theta}\Big|_{\theta=\theta_{old}}$$

- Converges much faster that gradient descent. In fact, from the Taylor expansion, we have

$$\frac{\partial J(\theta)}{\partial\theta} = \mathbf{H}(\theta-\theta^0)$$

$$\theta_{\mathrm{new}} = \theta_{old} - \mathbf{H}^{-1}(\mathbf{H}(\theta_{old}-\theta^0)) = \theta^0$$

- The minimum is found in one iteration.

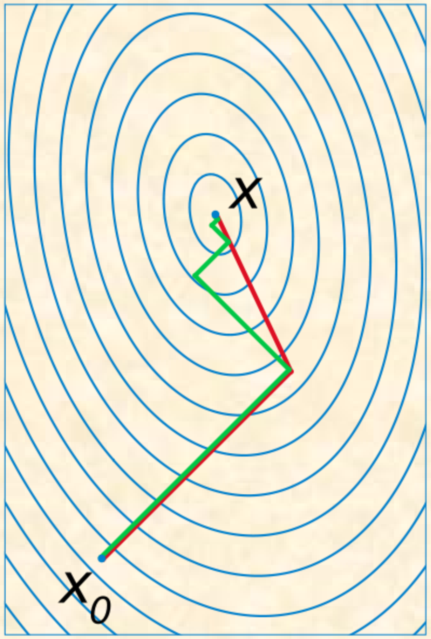


❖ Conjugate gradient method

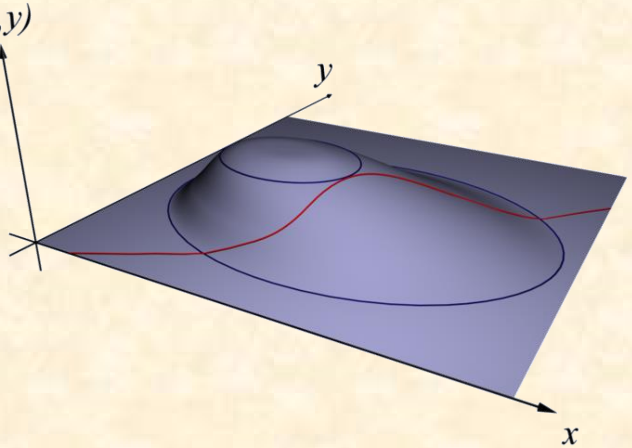
$$\Delta\theta_t = g_t - \beta_t\Delta\theta_{t-1}$$

$$\text{where } g_t = \frac{\partial J(\theta)}{\partial\theta}\Big|_{\theta=\theta_t}$$

$$\text{and } \beta_t = \frac{g_t^T g_t}{g_{t-1}^T g_{t-1}} \text{ or } \beta_t = \frac{g_t^T(g_t - g_{t-1})}{g_{t-1}^T g_{t-1}}$$



Constrained Optimization with Equality Constraints



Minimize J(θ)
subject to $f_i(\theta)=0$ for i=1, 2, …, m

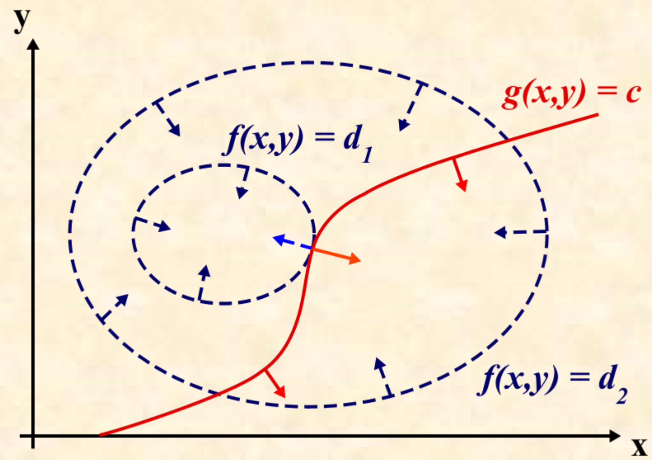
- Minimization happens at

$$\frac{\partial J(\theta)}{\partial \theta} = \lambda \frac{\partial f_i(\theta)}{\partial \theta}$$

- **Lagrange multipliers:** construct

$$L(\theta,\lambda) = J(\theta) - \sum_{i=1}^{m} \lambda_i f_i(\theta)$$

and solve $\dfrac{\partial L(\theta,\lambda)}{\partial \theta} = \dfrac{\partial L(\theta,\lambda)}{\partial \lambda} = 0$



Constrained Optimization with Inequality Constraints

Minimize $J(\theta)$ subject to $f_i(\theta) \geq 0$ for $i=1, 2, \ldots, m$

- $f_i(\theta) \geq 0$ $i=1, 2, \ldots, m$ defines a feasible region in which the answer lies.
- **Karush–Kuhn–Tucker (KKT) conditions:**

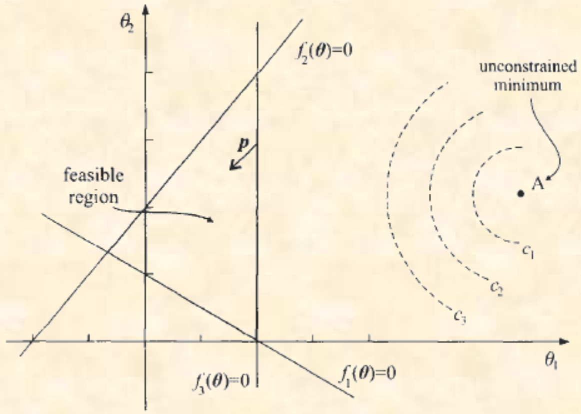
  A set of necessary conditions, which a local optimizer θ_* has to satisfy.

  There exists a vector λ of Lagrange multipliers such that

$$(1)\quad \frac{\partial}{\partial \boldsymbol{\theta}} L(\boldsymbol{\theta}_*, \boldsymbol{\lambda}) = 0$$

$$(2)\quad \lambda_i \geq 0 \text{ for } i = 1,2,\ldots,m$$

$$(3)\quad \lambda_i f_i(\boldsymbol{\theta}_*) = 0 \text{ for } i = 1,2,\ldots,m$$



(1) Most natural condition.
(2) $f_i(\theta_*)$ is inactive if $\lambda_i = 0$.
(3) $\lambda_i \geq 0$ if the minimum is on $f_i(\theta_*)$.
(4) The (unconstrained) minimum in the interior region if all $\lambda_i = 0$.
(5) For convex $J(\theta)$ and the region, local minimum is global minimum.
(6) Still difficult to compute. Assume some $f_i(\theta_*)$'s active, check $\lambda_i \geq 0$.

- **Convex function:**

$$f(\theta): S \subseteq \Re^l \to \Re \text{ is convax if } \forall \theta, \theta' \in S, \lambda \in [0,1]$$

$$f(\lambda\theta + (1-\lambda)\theta') \leq \lambda f(\theta) + (1-\lambda) f(\theta')$$

- **Concave function:**

$$f(\lambda\theta + (1-\lambda)\theta') \geq \lambda f(\theta) + (1-\lambda) f(\theta')$$

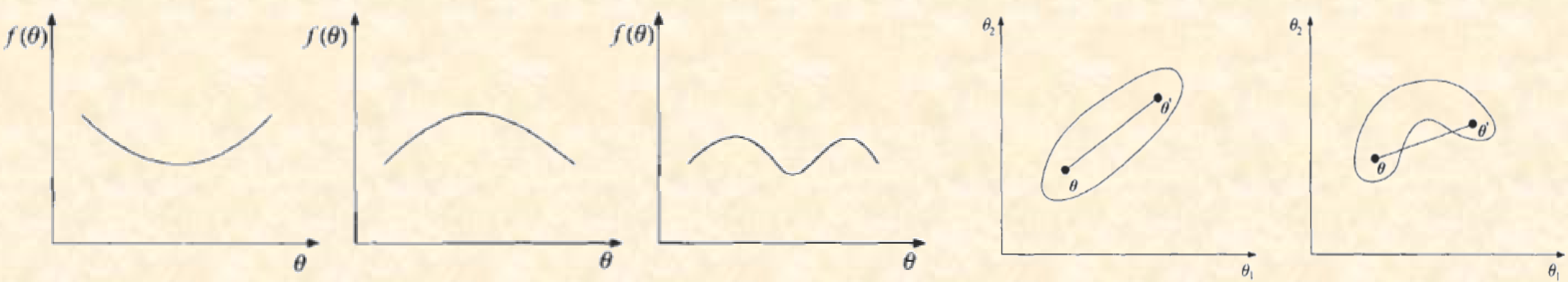
- **Convex set:**

$$S \subseteq \Re^l \text{ is a convax set if } \forall \theta, \theta' \in S, \lambda \in [0,1]$$

$$\lambda\theta + (1-\lambda)\theta') \in S$$

Local minimum of a convex function is also global minimum.

If $f(\theta)$ is concave, then $X = \{\theta \mid f(\theta) \geq b\}$ is a convex set.



❖ Min-Max duality

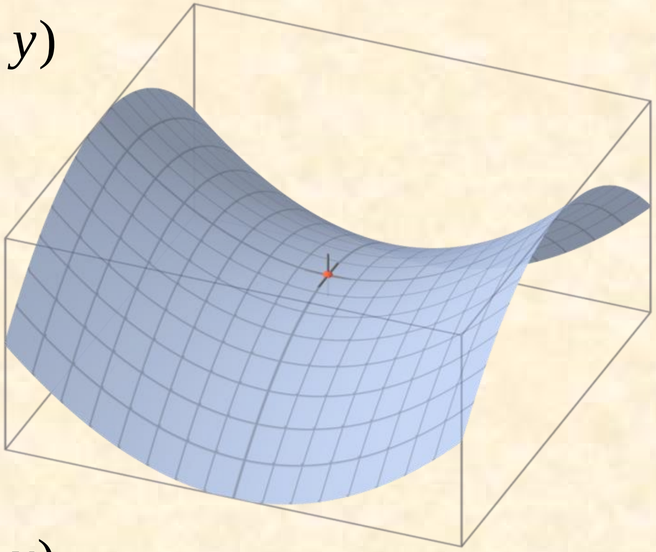
Game : A pays $F(x, y)$ \$ to B while A chooses x and B chooses y

A's goal : $\min_x \max_y F(x, y)$, B's goal : $\max_y \min_x F(x, y)$

The two problems are dual to each other.

In general : $\min_x F(x, y) \le F(x, y) \le \max_y F(x, y)$

Therefore, $\max_y \min_x F(x, y) \le \min_x \max_y F(x, y)$



Saddle point condition :

If there exists (x_*, y_*) such that

$F(x_*, y) \le F(x_*, y_*) \le F(x, y_*)$

or equivalent ly :

$F(x_*, y_*) = \max_y \min_x F(x, y) = \min_x \max_y F(x, y)$

❖ Lagrange duality

- Recall the optimization problem:

$$\text{Minimize} \quad J(\theta) \qquad \text{s.t. } f_i(\theta) \ge 0 \text{ for } i = 1,2,\dots,m$$

$$\text{Lagrange function } : L(\theta,\lambda) = J(\theta) - \sum_{i=1}^{m} \lambda_i f_i(\theta)$$

Because $\max_{\lambda \ge 0} L(\theta,\lambda) = J(\theta)$, we have

$$\min_{\theta} J(\theta) = \min_{\theta} \max_{\lambda \ge 0} L(\theta,\lambda)$$

- Convex Programming

For a large class of applicatio ns, $J(\theta)$ is convex, $f_i(\theta)$'s are concave then, the minimizati on solution (θ_*, λ_*) is a saddle point of $L(\theta,\lambda)$

$$L(\theta_*,\lambda) \le L(\theta_*,\lambda_*) \le L(\theta,\lambda_*)$$

$$L(\theta_*,\lambda_*) = \min_{\theta} \max_{\lambda \ge 0} L(\theta,\lambda) = \max_{\lambda \ge 0} \min_{\theta} L(\theta,\lambda)$$

Therefore, the optimizati on problem becomes $\max_{\lambda \ge 0} \min_{\theta} L(\theta,\lambda)$, or

$$\max_{\lambda \ge 0} L(\theta,\lambda) \qquad \text{subject to } \frac{\partial}{\partial \theta} L(\theta,\lambda) = 0$$

MUCH SIMPLER!

Mercer's Theorem and the Kernel Method

- Mercer's theorem:

  Let $x \in \Re^l$ and given a mapping $\phi(x) \in H$,

  (H denotes Hilbert space, i.e. finite or infinite Euclidean space)

  the inner product $\langle \phi(x), \phi(y) \rangle$ can be expressed as a **kernel function**

  $$\langle \phi(x), \phi(y) \rangle = K(x, y)$$

  where $K(x, y)$ is symmetric, continuous, and positive semi-definite.

  The opposite is also true.

The kernel method can transform any algorithm that solely depends on the dot product between two vectors to a kernelized vesion, by replacing dot product with the kernel function. The kernelized version is equivalent to the algorithm operating in the range space of φ. Because kernels are used, however, φ is never explicitly computed.