10-701 Cheat Sheet

Non-Parametric

MaxLikelihood learning window will give you delta functions, which is a kind of over fitting. Use Leave-one-out cross validation for model selection. Idea: Use some of the data to estimate density; Use other part to evaluate how well it works. Pick the parameter that works best.
$\log p(x_i|X\setminus\{x_i\}) = \log \frac{1}{n-1}\sum_{j\neq i} k(x_i,x_j)$, the sum over all points is $\frac{1}{n}\sum_{i=1}^n \log\left[\frac{n}{n-1}p(x_i) - \frac{1}{n-1}k(x_i,x_i)\right]$ where $p(x) = \frac{1}{n}\sum_{i=1}^n k(x_i,x)$.
why must we not check too many parameters? that you can overfit more; for a given dataset, a few particular parameter values might happen to do well in k-fold CV by sheer chance, where if you had a new dataset they might not do so well. Checking a reasonable number of parameter values makes you less likely to hit those "lucky" spots helps mitigate this risk.
Silverman's Rule for kernel size Use average distance from k nearest neighbors $r_i = \frac{r}{k}\sum_{x\in \mathrm{NN}(x_i,k)}\|x_i - x\|$.
Watson Nadaraya 1. estimate $p(x|y=1)$ and $p(x|y=-1)$; 2. compute by Bayes rule
$p(y|x) = \frac{p(x|y)p(y)}{p(x)} = \frac{\frac{1}{m_y}\sum_{y_i=y} k(x_i,x)\cdot\frac{m_y}{m}}{\frac{1}{m}\sum_i k(x_i,x)}$. 3. Decision boundary
$p(y=1|x) - p(y=-1|x) = \frac{\sum_j y_j k(x_j,x)}{\sum_i k(x_i,x)} = \sum_j y_j \frac{k(x_j,x)}{\sum_i k(x_i,x)}$
Actually, we assume that p(x—y) is equal to $1/m_y * \sum_y k(x_i,x)$. Using this definition, we can see $p(x,-1)+p(x,1) = p(x|-1)p(-1)+p(x|1)p(1) = p(x)$.
This can be incorporated into the regression framework in chap 6 of PRML. Where we define $f(x-x_n, t\neq t_n) = 0$, and $f(x-x_n, t=t_n) = f(x-x_n)$. Using this definition, we can derive all the probabilities on this slide. (see my handwritten notes on chap 6 of PRML).
Regression case is the same equation.
kNN Let optimal error rate be p. Given unlimited **iid** data, 1NN's error rate is $\leq 2p(1-p)$.

Matrix Cookbook

$\frac{\partial \boldsymbol{x}^T\boldsymbol{a}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{a}^T\boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{a}$
$\frac{\partial \boldsymbol{a}^T\boldsymbol{X}\boldsymbol{b}}{\partial \boldsymbol{X}} = \boldsymbol{a}\boldsymbol{b}^T$, $\frac{\partial \boldsymbol{a}^T\boldsymbol{X}^T\boldsymbol{b}}{\partial \boldsymbol{X}} = \boldsymbol{b}\boldsymbol{a}^T$, $\frac{\partial \boldsymbol{a}^T(\boldsymbol{X}^T|\boldsymbol{X})\boldsymbol{a}}{\partial \boldsymbol{X}} = \boldsymbol{a}\boldsymbol{a}^T$
$W\in\boldsymbol{S}$, $\frac{\partial}{\partial \boldsymbol{s}}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})^T\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s}) = -2\boldsymbol{A}^T\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})$,
$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{x}-\boldsymbol{s})^T\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{s}) = 2\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{s})$,
$\frac{\partial}{\partial \boldsymbol{s}}(\boldsymbol{x}-\boldsymbol{s})^T\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{s}) = -2\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{s})$,
$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})^T\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s}) = 2\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})$,
$\frac{\partial}{\partial \boldsymbol{A}}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})^T\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s}) = -2\boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})\boldsymbol{s}^T$.
$\mathrm{Tr}(\boldsymbol{A}) = \sum_i \boldsymbol{A}_{ii}$. For two equal sized matrices, $\mathrm{Tr}(\boldsymbol{A}^T\boldsymbol{B}) = \mathrm{Tr}(\boldsymbol{B}^T\boldsymbol{A}) = \mathrm{Tr}(\boldsymbol{A}\boldsymbol{B}^T) = \mathrm{Tr}(\boldsymbol{B}\boldsymbol{A}^T) = \sum_{i,j}\boldsymbol{A}_{ij}\boldsymbol{B}_{ij}$.
$\mathrm{Tr}(\boldsymbol{A}) = \mathrm{Tr}(\boldsymbol{A}^T), \mathrm{Tr}(\boldsymbol{A}+\boldsymbol{B}) = \mathrm{Tr}(\boldsymbol{A}) + \mathrm{Tr}(\boldsymbol{B})$. For square matricis,
$\mathrm{Tr}(\boldsymbol{A}\boldsymbol{B}) = \mathrm{Tr}(\boldsymbol{B}\boldsymbol{A}), \mathrm{Tr}(\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}) = \mathrm{Tr}(\boldsymbol{C}\boldsymbol{A}\boldsymbol{B}) = \mathrm{Tr}(\boldsymbol{B}\boldsymbol{C}\boldsymbol{A})$ (trace rotation).

Classifers and Regressors

Naive Bayes Conditionally independent:
$P(x_1,x_2,\ldots|C) = \prod_i P(x_i|C)$. One way to avoid divide by zero: add (1,1,.....,1) and (0,0,.....,0) to both classes
Learns $P(x_i|y)$ for *Discrete* x_i – $P(x_i|y) = \frac{\#D(X_i=x_i,Y=y)}{\#D(Y=y)}$
For smoothing, use $P(x_i|y) = \frac{\#D(X_i=x_i,Y=y)+k}{\#D(Y=y)+n_i k}$, where n_i is the number of different possible values for X_i (In practice problem set, Jing Xiang used $k=1$?) *Continuous* x_i – Can use any PDF, but usually use Gaussian
$P(x_i|y) = \mathcal{N}(\mu_{X_i|y}, \sigma^2_{X_i|y})$, where $\mu_{X_i|y}$ and $\sigma_{X_i|y}$ are, respectively, the average and variance of X_i for all data points where $Y=y$. The Gaussian distribution already provides smoothing.
Perceptron Produces linear decision boundaries. *Classifies* using $\hat{y} = X_{test}\,w + b$ *Learns* w and b by updating w whenever $y_i(w^Tx_i+b)\leq 0$ (i.e. incorrectly classified). Updates as $w\leftarrow w + x_iy_i, b\leftarrow b+y_i$ Repeat until all examples are correctly classified. w is some linear combination $\sum_i \alpha_i x_i(y_i * x_i)$ of data points, and decision boundary is the linear hyperplane $f(x) = w^Tx + b$. **Note** that the perceptron is the same as stochastic gradient descent with a hinge loss function of $max(0, 1-y_i[<w,x_i>+b])$ (**we can't remove 1 in the loss function; otherwise we can set** $w, b = 0$).
Convergence of perceptron proof 1 Here we use a perceptron without b. Assume we have $\boldsymbol{w}^*$ that has margin γ $(\min(\boldsymbol{w}^*)^Ty_ix_i = \gamma$), and $\|\boldsymbol{w}^*\| = 1, \|x_i\| = 1$. We start from $\boldsymbol{w}_0 = 0$. Assume that we have made M mistakes. We have 1) $\boldsymbol{w}_M\cdot\boldsymbol{w}^* = (\boldsymbol{w}_{M-1} + y_ix_i)\cdot\boldsymbol{w}^* \geq \boldsymbol{w}_{M-1}\cdot\boldsymbol{w}^* + \gamma$. So we have $\boldsymbol{w}_M\cdot\boldsymbol{w}^* \geq M\gamma$.
2) $\boldsymbol{w}_M\cdot\boldsymbol{w}_M = (\boldsymbol{w}_{M-1}+y_ix_i)\cdot(\boldsymbol{w}_{M-1}+y_ix_i) = \boldsymbol{w}_{M-1}\cdot\boldsymbol{w}_{M-1} + 2y_ix_i\cdot\boldsymbol{w}_{M-1} + (y_ix_i)\cdot(y_ix_i) \leq \boldsymbol{w}_{M-1}\cdot\boldsymbol{w}_{M-1} + 1$. So we have $\boldsymbol{w}_M\cdot\boldsymbol{w}_M < M$.
Combining them, using Cauchy-Schwarz, we have $M\gamma \leq \boldsymbol{w}_M\cdot\boldsymbol{w}^* \leq \|\boldsymbol{w}_M\|\|\boldsymbol{w}^*\| \leq \sqrt{M}$. So $M\leq 1/\gamma^2$. **proof 2** Let potential function $Q_i = \|\boldsymbol{w}_i\| - \boldsymbol{w}_i\cdot\boldsymbol{w}^*$, where i is the number of iterations. Assuming up to iteration i, we have M mistakes, so we have $Q_i \leq \sqrt{M} - M\gamma$. Clearly $Q_i\geq 0$ by Cauchy-Schwarz. So we have $\sqrt{M} - M\gamma \geq 0$.

Kernel

Kernel function $k(\boldsymbol{x},\boldsymbol{x}') = \phi(\boldsymbol{x})^T\phi(\boldsymbol{x}')$ for some $\phi(\cdot)$. For a set of data points $\{\boldsymbol{x}_i\}$, we have Gram matrix (kernel matrix) $K_{ij} = k(\boldsymbol{x}_i,\boldsymbol{x}_j)$. A **necessary and sufficient** condition for being a valid kernel function: K always positive semidefinite. Proof: $\boldsymbol{\alpha}^TK\boldsymbol{\alpha} = \sum_{ij}\alpha_i\alpha_jK_{ij} = \sum_{ij}\alpha_i\alpha_j\langle\phi(\boldsymbol{x}_i),\phi(\boldsymbol{x}_j)\rangle = \langle\sum_i\alpha_i\phi(\boldsymbol{x}_i), \sum_j\alpha_j\phi(\boldsymbol{x}_j)\rangle \geq 0$.
Mercer's Theorem for any symmtric function $k:\mathcal{X}\times\mathcal{X}\to\mathbb{R}$ which is square integrable and satisfying $\int_{\mathcal{X}\times\mathcal{X}} k(x,x')f(x)f(x')\mathrm{d}x\mathrm{d}x' \geq 0$ for $f\in L_2(\mathcal{X})$, we have a feature space $\Phi(x)$ and $\boldsymbol{\lambda}\geq 0$ that $k(x,x') = \sum_i\lambda_i\phi_i(x)\phi_i(x')$.
new kernel from old ones Given kernels $k_1(x,x'), k_2(x,x')$, $ck_1(x,x')$, $f(x)k_1(x,x')f(x')$, $k_1(x,x') + k_2(x,x')$, $k_1(x,x')k_2(x,x')$ are new valid kernels. Proof: 1) write the kernel as the dot product of two vectors; 2) use Mercer's Theorem; 3) any Gram matrix derived from it is positive semidefinite. $k_1(x,x') - k_2(x,x')$ is **invalid**: let $k_1(x,x') = 1$ for $x = x'$, and 0 otherwise, and $k_2(x,x') = 2k_1(x,x')$. The Gram matrix of new kernel is not PSD.
PSD matrices Products of two PSD matrices are not always PSD. Let A be 2×2 PSD, and B be $\mathrm{diag}(1,2)$. AB is not PSD (columns scaled differently). **PSD's eigen decomposition** $A = UDU^T$. $A^{m+1} = AA^m = UDU^T(UD^mU^T) = UD(U^TU)D^mU^T = UD^{m+1}U^T$. **Any**
PSD is a covariance matrix Let $\boldsymbol{x}$ be a random vector with covariance I, PSD Q is the covariance matrix for $Q^{1/2}\boldsymbol{x}$: $\mathrm{cov}(Q^{1/2}\boldsymbol{x}) = Q^{1/2}\mathrm{cov}(\boldsymbol{x})Q^{1/2} = Q^{1/2}Q^{1/2} = Q$.
examples polynomial: $(\langle x,x'\rangle + c)^d, c\geq 0$. For $c=0$, it's a polynomial having all terms of order d; for $c>0$, it contains all terms of order up to d.

Convexity

Convex Sets
Definition: A set C is *convex* if the line segment between any two points in C lies in C, i.e. if for any $x_1, x_2\in C$ and any θ with $0\leq\theta\leq 1$, we have

$$\theta x_1 + (1-\theta)x_2 \in C$$

Examples:

- Empty set $\emptyset$, single point x_0, the whole space $\mathbb{R}^n$
- Hyperplane $\{x|a^Tx = b\}$, halfspaces $\{x|a^Tx\leq b\}$
- Euclidean balls $\{x|\|x-x_c\|_2\leq r\}$
- Positive semidefinite marices $S^n_+ = \{A\in S^n|A\succeq 0\}$ (S^n is the set of symmetric $n\times n$ matrices)

Convexit preserving set operations:

- Translation $\{x+b|x\in C\}$
- Scaling $\{\lambda x|x\in C\}$
- Affine function $\{Ax+b|x\in C\}$
- Intersection $C\cap D$
- Set sum $C+D = \{x+y|x\in C, y\in D\}$

Convex Functions
Definition: A function $f:\mathbb{R}^n\to\mathbb{R}$ is *convex* if $\mathbf{dom}f$ is a convex set and if for all x, $y\in\mathbf{dom}f$, and θ with $0\leq\theta\leq 1$, we have

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta)f(y)$$

First-order conditions: Suppose f is differentiable. Then f is convex if and only if $\mathbf{dom}f$ is convex and

$$f(y)\geq f(x) + \bigtriangledown f(x)^T(y-x)$$

Second-order conditions: Assume that f is twice differentiable. Then f is convex if and only if $\mathbf{dom}f$ is convex and its Hessian is positive semidefinite: for all $x\in\mathbf{dom}f$,

$$\bigtriangledown^2 f(x)\succeq 0$$

Strictly convex: Whenever $x\neq y$ and $0<\theta<1$, we have

$$f(\theta x + (1-\theta)y) < \theta f(x) + (1-\theta)f(y)$$

Or

$$f(y) > f(x) + \bigtriangledown f(x)^T(y-x)$$

Or **sufficient but not necessary condition:**

$$\bigtriangledown^2 f(x)\succ 0$$