Advanced Linear Regression: Bayesian, Kernel and Online

(Jan 11th, 2017)

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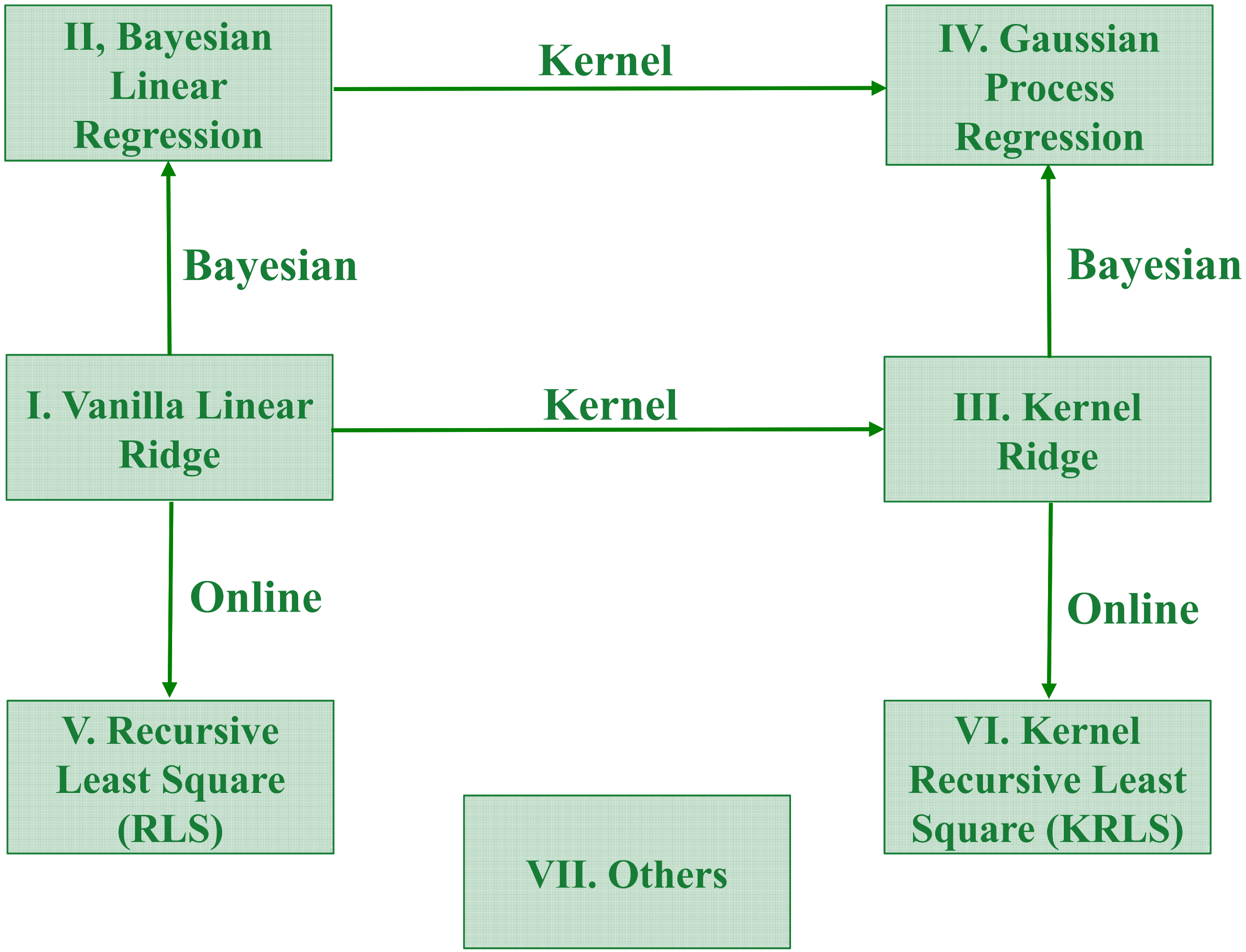
Outline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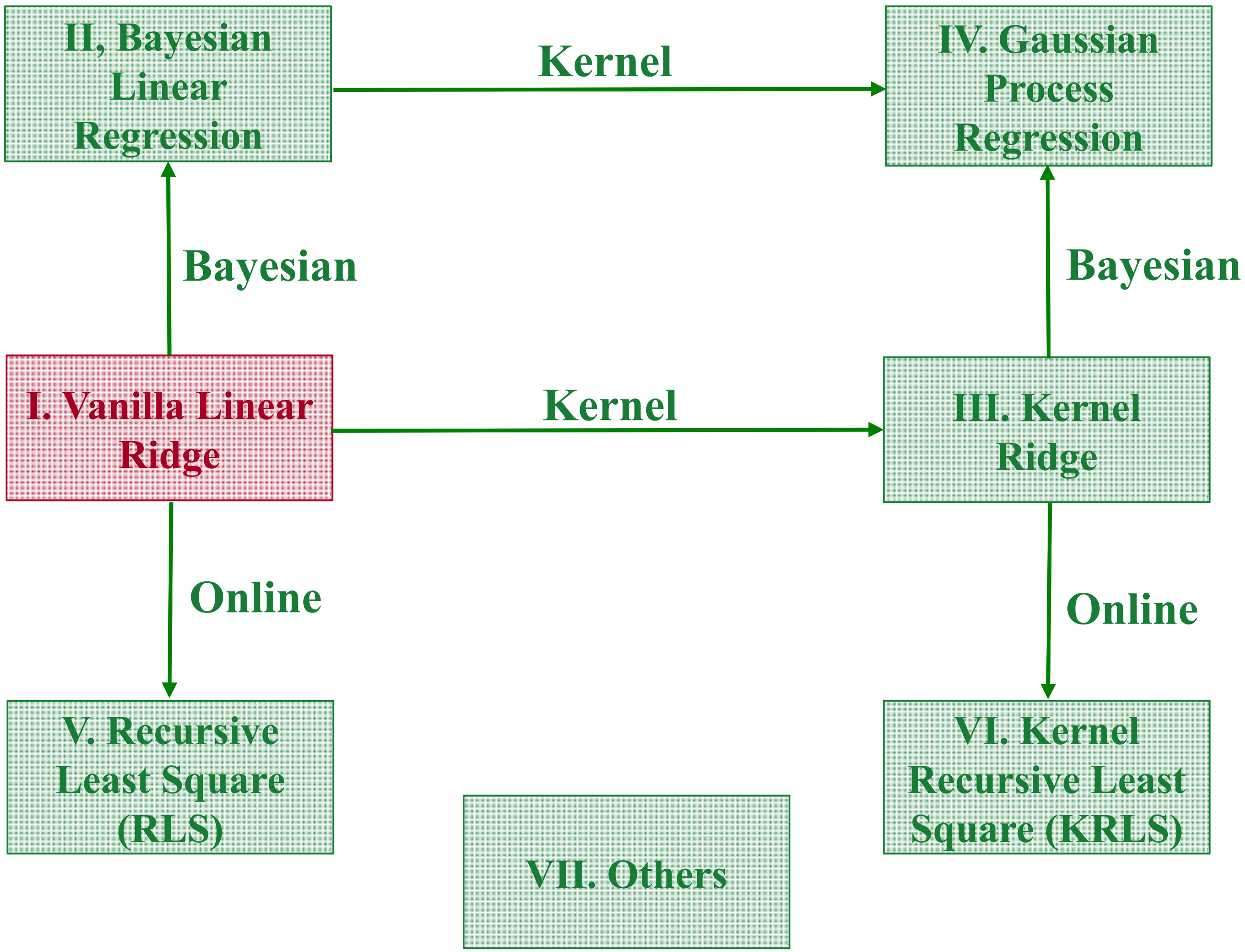
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• I. Vanilla Linear Ridge

- **Matrix Form**

$$\underset{n\times m}{Y} = \underset{n\times d}{X}\cdot \underset{d\times m}{W} + e$$

$d \to$ features

$m \to$ multiple output

$$\text{loss} = \|e\|^2 = \|Y - XW\|^2 = (Y-XW)^T(Y-XW)$$

$$= Y^TY - Y^TXW - W^TX^TY + W^TX^TXW$$

$$\frac{\partial}{\partial W}\text{loss} = -2X^TY + 2X^TXW = 0$$

$$\boxed{W = (X^TX)^{-1}X^TY = X^{+}Y}$$

$\to$ pseudo-inverse

• I. Vanilla Linear Ridge

- **Ridge**

$$loss = \|y - Xw\|^2 + \lambda \|w\|^2$$

$$\frac{\partial}{\partial w} loss = -2X^T y + 2X^T X w + 2\lambda w = 0$$

$$\boxed{w = (X^T X + \lambda I_d)^{-1} X^T y}$$

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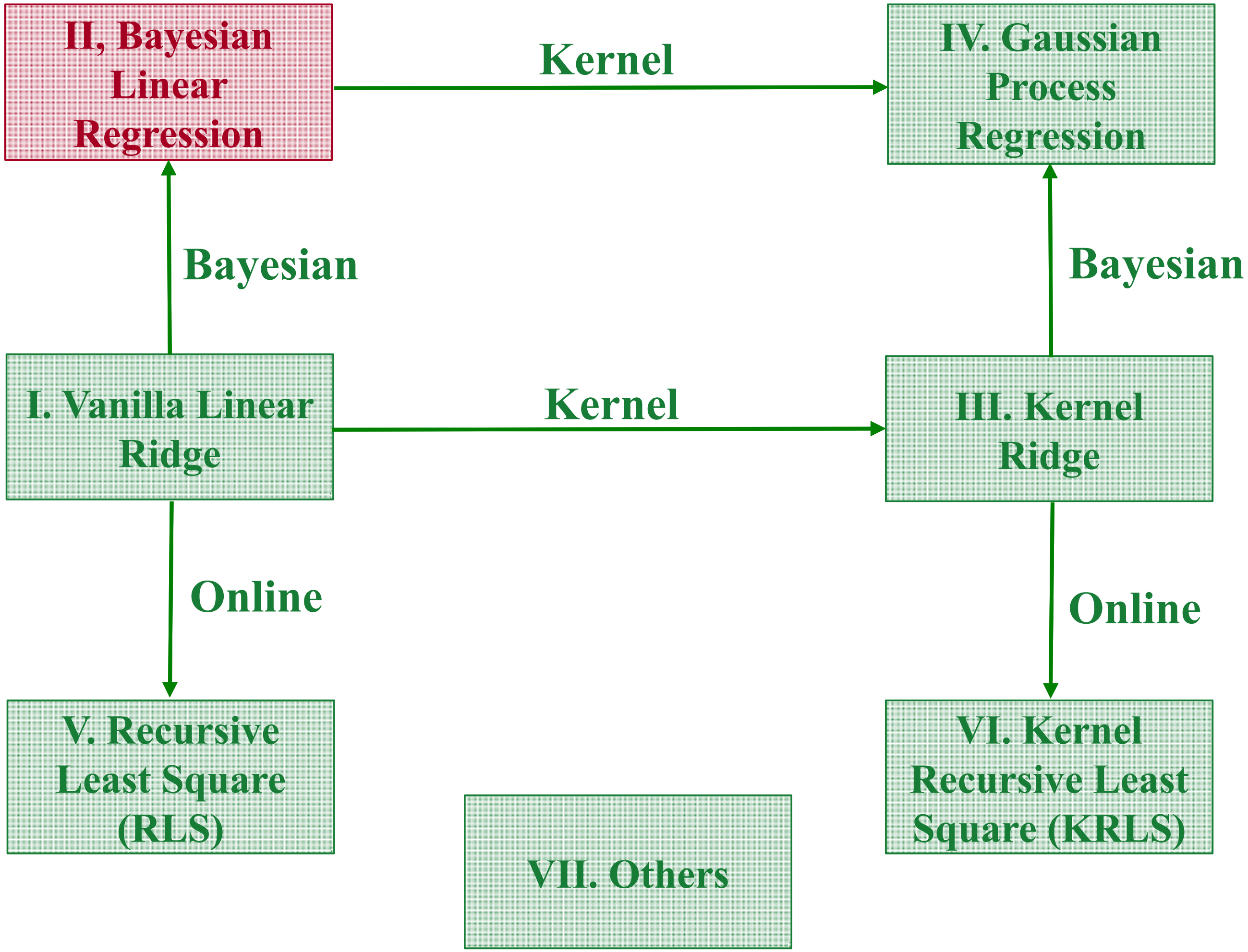
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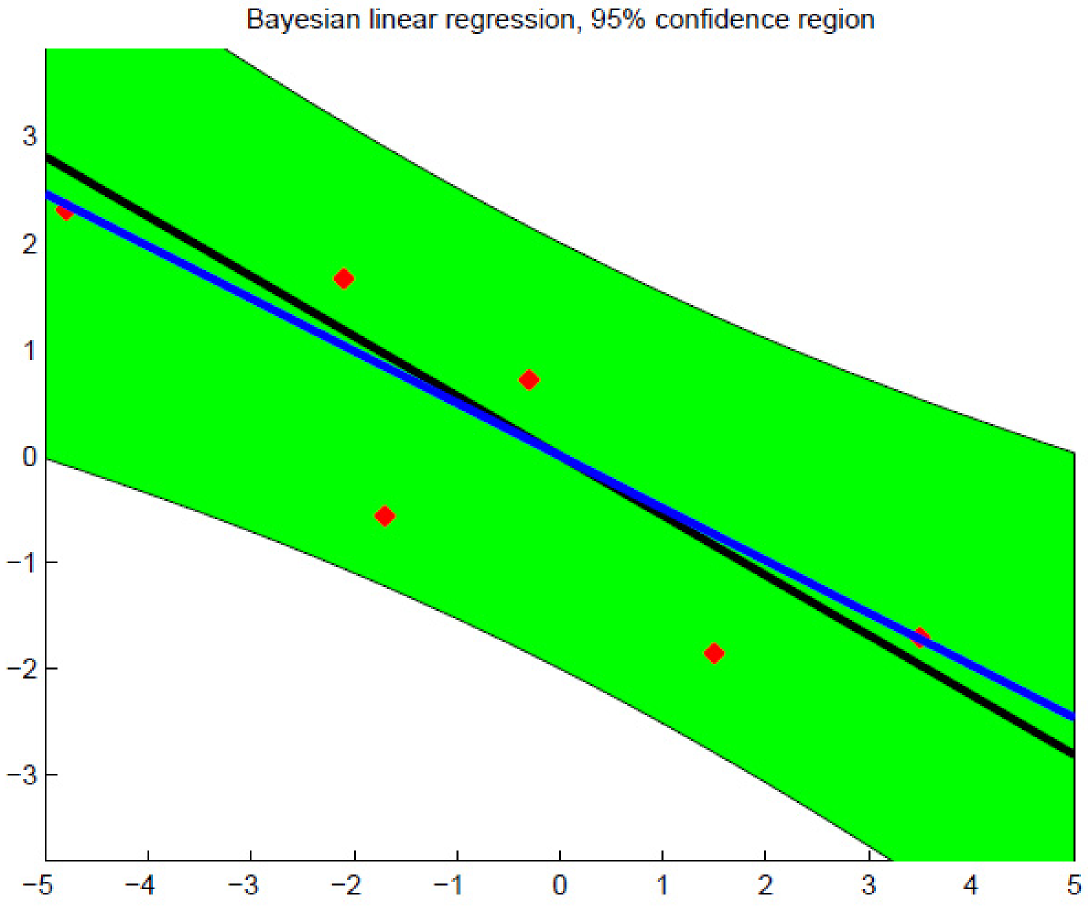
• II, Bayesian Linear Regression

- **Effect of Bayesian**



• II, Bayesian Linear Regression

- **Bayesian Interpretation**

For simplity, $m=1$ (single target)

$$\underset{n\times 1}{\underline{y}} = \underset{n\times d}{\underline{X}}\,\underset{d\times 1}{\underline{w}} + \underset{n\times 1}{\underline{\varepsilon}}, \quad \boxed{\varepsilon_i \sim N(0, \delta^2)}$$

$$\Rightarrow y \sim N(Xw, \delta^2 I_n)$$

Plus, we assume:

$$\boxed{w \sim N(0, \tau^2 I_d)}$$

• II, Bayesian Linear Regression

- **Posterior**

$$p(w \mid X, y) \propto P(X, y \mid w)\, P(w)$$

$$\propto \exp\Big(\underbrace{-\frac{(y-Xw)^T(y-Xw)}{2\delta^2} - \frac{w^T w}{2\tau^2}}_{\downarrow\ +\ \text{const}\quad (w-\mu)^T \Lambda (w-\mu)}\Big)$$

$$\Lambda_{d\times d} = \Big(\frac{1}{\delta^2} X^T X + \frac{1}{\tau^2} I_d\Big)$$

$$\mu = \frac{1}{\delta^2} \Lambda^{-1} X^T y = \Big(X^T X + \frac{\delta^2}{\tau^2} I\Big) X^T y$$

$$\boxed{P(w \mid D) \sim \mathcal{N}(\mu, \Lambda)}$$

MAP : $w = \mu$

$\Leftrightarrow$ ridge

• II, Bayesian Linear Regression

- **Predictive (1)**

$()_{d\times 1}$ $\rightarrow$ Scalar

Given a new sample (x_0, y_0)

We want

$$\underline{P(y_0 \mid x_0, D)}, \quad D = \{(x_1, y_1), \cdots, (x_n, y_n)\}$$

Use Bayesian Average :

$$P(y_0 \mid x_0, D) = \int P(y_0, w \mid x_0, D)\, dw$$

$$= \int \underbrace{P(y_0 \mid x_0, D, w)}_{P(y_0 \mid x_0, w)} \underbrace{P(w \mid x_0, D)}_{P(w \mid D)}\, dw$$

$y_0 \perp D \mid w$ $\qquad$ $w \perp x_0 \mid D$

$$= \int N(w^T x_0, \delta^2)\, N(\mu, \Lambda^{-1})\, dw$$

• II, Bayesian Linear Regression

- **Predictive (2)**

$$p(y_0|x_0,D) \propto \int \exp\Big(\underbrace{\frac{(y_0-w^Tx_0)^2}{2\delta^2} - \frac{1}{2}(w-u)^T\Lambda(w-u)}_{(w-m)^TL(w-m)+\cdots}\Big)dw$$

Our goal:

$$\int g(y_0)\cdot N(w|\ldots)\,dw = g(y_0)$$

$$p(y_0|x_0,D) \propto \int \exp\Big(\frac{(w-m)^TL(w-m)}{2}\Big)\underbrace{\exp\Big(\frac{m^TLm}{2} - \frac{y_0^2}{2\delta^2}\Big)}_{g(y_0)}dw$$

$$\boxed{\begin{aligned} g(y_0) &= \exp\Big(-\frac{\lambda}{2}(y_0-\hat{y}_0)^2\Big) \\ \hat{y}_0 &= u^Tx_0 \\ \frac{1}{\lambda} &= \delta^2 + x_0^T\Lambda^{-1}x_0 \end{aligned}}$$

$$\boxed{\begin{aligned} L &= \frac{x_0x_0^T}{\delta^2} + \Lambda \\ m &= L^{-1}\Big(\frac{y_0x_0}{\delta^2} + \Lambda u\Big) \end{aligned}}$$

• II, Bayesian Linear Regression

- **Predictive (3)**

Same !

$$N(y_0 \mid x_0, D) \sim N(u^T x_0, \delta^2 + x_0^T \Lambda^{-1} x_0)$$

$$\varepsilon_i \sim N(0, \delta^2)$$

$$\omega \sim N(0, \tau^2 I_d)$$

$$u = (X^T X + \frac{\delta^2}{\tau^2} I) X^T y$$

$$\Lambda = \frac{1}{\delta^2} X^T X + \frac{1}{\tau^2} I_d$$

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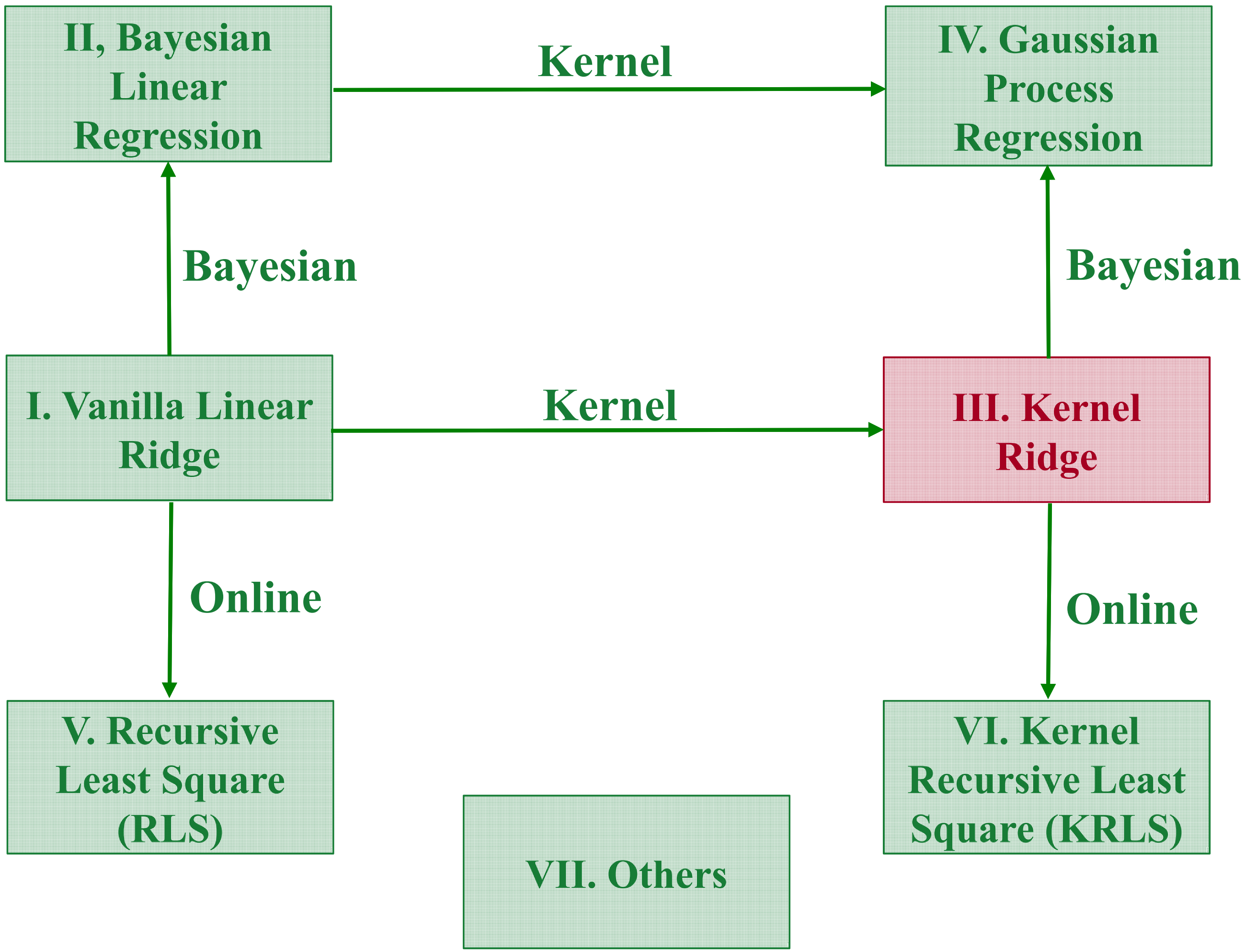
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• III. Kernel Ridge

- **Dual Form**

$$(X^T X + \lambda I) w = X^T y$$

$$\lambda w = X^T (y - Xw)$$

$$w = X^T \cdot \boxed{\frac{y - Xw}{\lambda}} \stackrel{\text{def}}{=} w = X^T \alpha$$

$$\boxed{\begin{array}{l}\text{the optimal } w \text{ is} \\ \quad \text{the linear combination of } X\end{array}}$$

• III. Kernel Ridge

- **Kernelized Ridge**

$\overset{def}{=} K$

$\nearrow$ or: $K = \phi^T(X)\,\phi(X)$

$$\omega = X^T \alpha$$

$$y = Xw + e = \underbrace{X \cdot X^T}\alpha + \varepsilon$$

$$L_2 = \|\varepsilon\|_2 + \lambda \|w\|_2 = (y - K\alpha)^T (y - K\alpha) + \lambda \alpha^T \underbrace{XX^T}_{\to K} \alpha$$

$$L_2 = y^T y - \alpha^T K^T y - y^T K \alpha + \alpha^T K^T K \alpha + \lambda \alpha^T K \alpha$$

$$\frac{\partial}{\partial \alpha} L_2 = -2K^T y + 2K^T K \alpha + 2\lambda K^T = 0$$

$$\Rightarrow \boxed{\alpha = (K + \lambda I_n)^{-1} y}$$

• III. Kernel Ridge

- **Big-O Analysis**

For a new entry x

$$\underset{1\times m}{\underline{y}} = \underset{1\times n}{\underline{K(x, X)}} \cdot \underset{n\times m}{\underline{\alpha}} + \varepsilon$$

	Linear Ridge	Kernel Ridge
Training Time	$O\left(d^3 + Nd^2\right)$	$O\left(N^3\right)$
Predicting Time	$O(d)$	$O(d)$
Model Size	$O(d)$	$O(d) + O(Nd) = O(Nd)$

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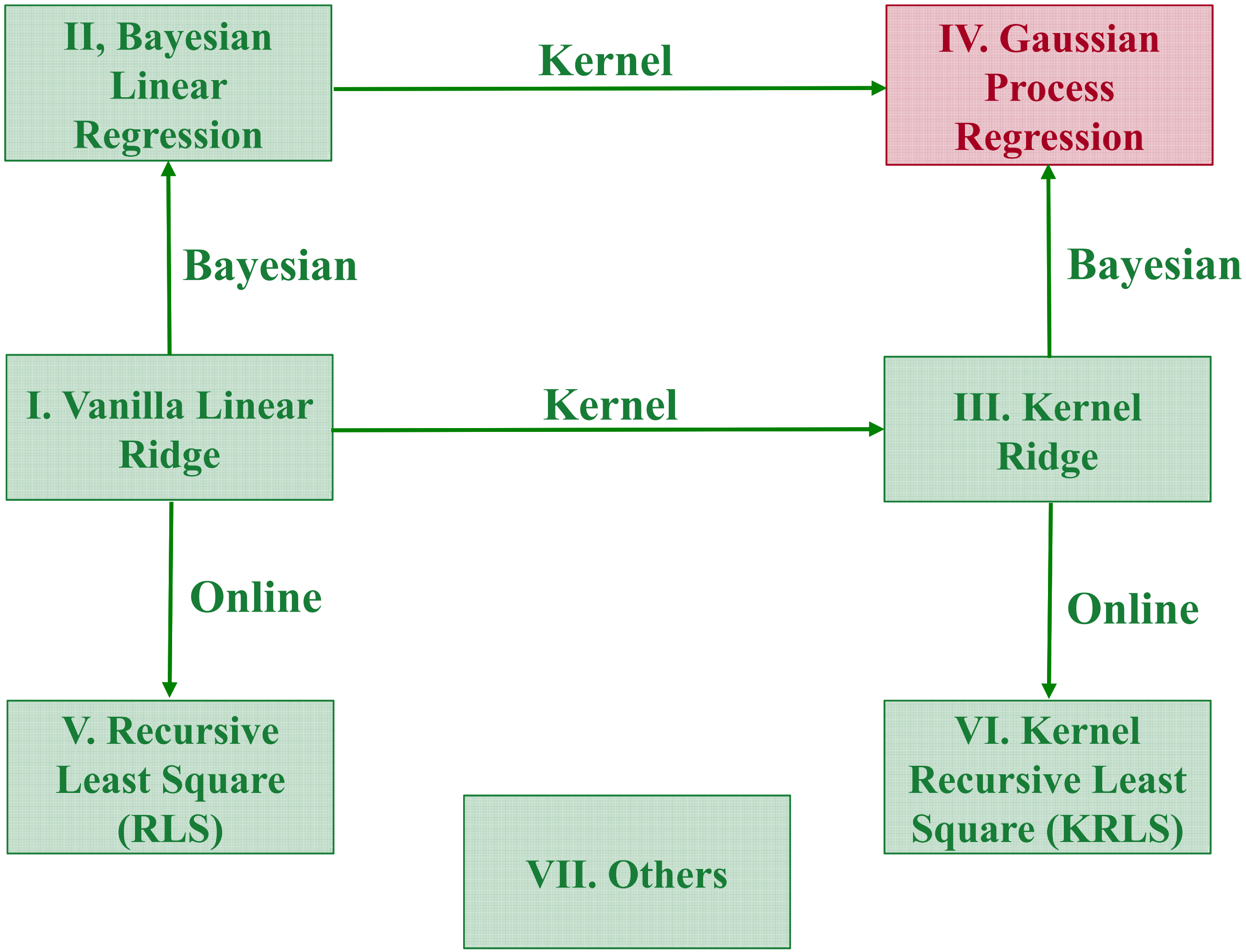
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• IV. Gaussian Process Regression

- **Idea**

a) Kernel as Covariance function

$$k(x, x') = \sigma_f^2 \exp\left[\frac{-(x-x')^2}{2l^2}\right] + \sigma_n^2 \delta(x, x')$$

$$K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_n) \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \cdots & k(x_n, x_n) \end{bmatrix}$$

$$K_* = \begin{bmatrix} k(x_*, x_1) & k(x_*, x_2) & \cdots & k(x_*, x_n) \end{bmatrix} \qquad K_{**} = k(x_*, x_*)$$

b) Sample from a multivariate Gaussian

$$\begin{bmatrix} \mathrm{y} \\ y_* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} K & K_*^{\mathrm{T}} \\ K_* & K_{**} \end{bmatrix}\right)$$

$$y_* | \mathrm{y} \sim \mathcal{N}(K_* K^{-1} \mathrm{y},\ K_{**} - K_* K^{-1} K_*^{\mathrm{T}})$$

c) Fit the **distribution of functions**

• IV. Gaussian Process Regression

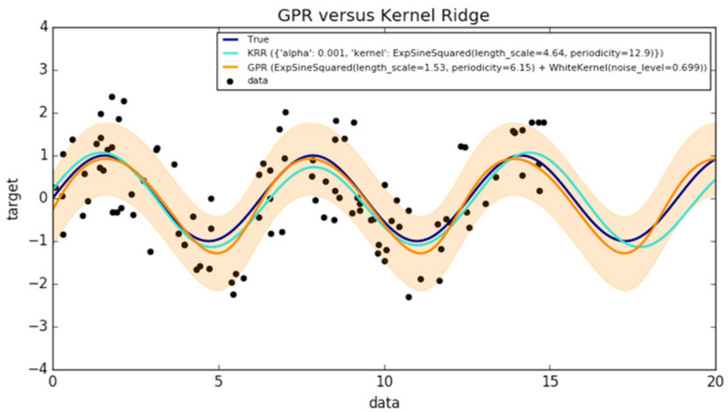
- **Hyperparameter as Optimization**

a) Use Conjugate Gradients or other optimizer to optimize the likelihood => **Bayesian Optimization**

$$\theta = \{l, \sigma_f, \sigma_n\}$$

$$\log p(\mathrm{y}|\mathrm{x}, \theta) = -\frac{1}{2}\mathrm{y}^{\mathrm{T}}K^{-1}\mathrm{y} - \frac{1}{2}\log|K| - \frac{n}{2}\log 2\pi$$

b) GPR and Kernel Ridge



- *Time for KRR fitting: 10.243*
- *Time for GPR fitting: 0.223*
- *Time for KRR prediction: 0.083*
- *Time for GPR prediction: 0.091*
- *Time for GPR prediction with standard-deviation: 0.386*

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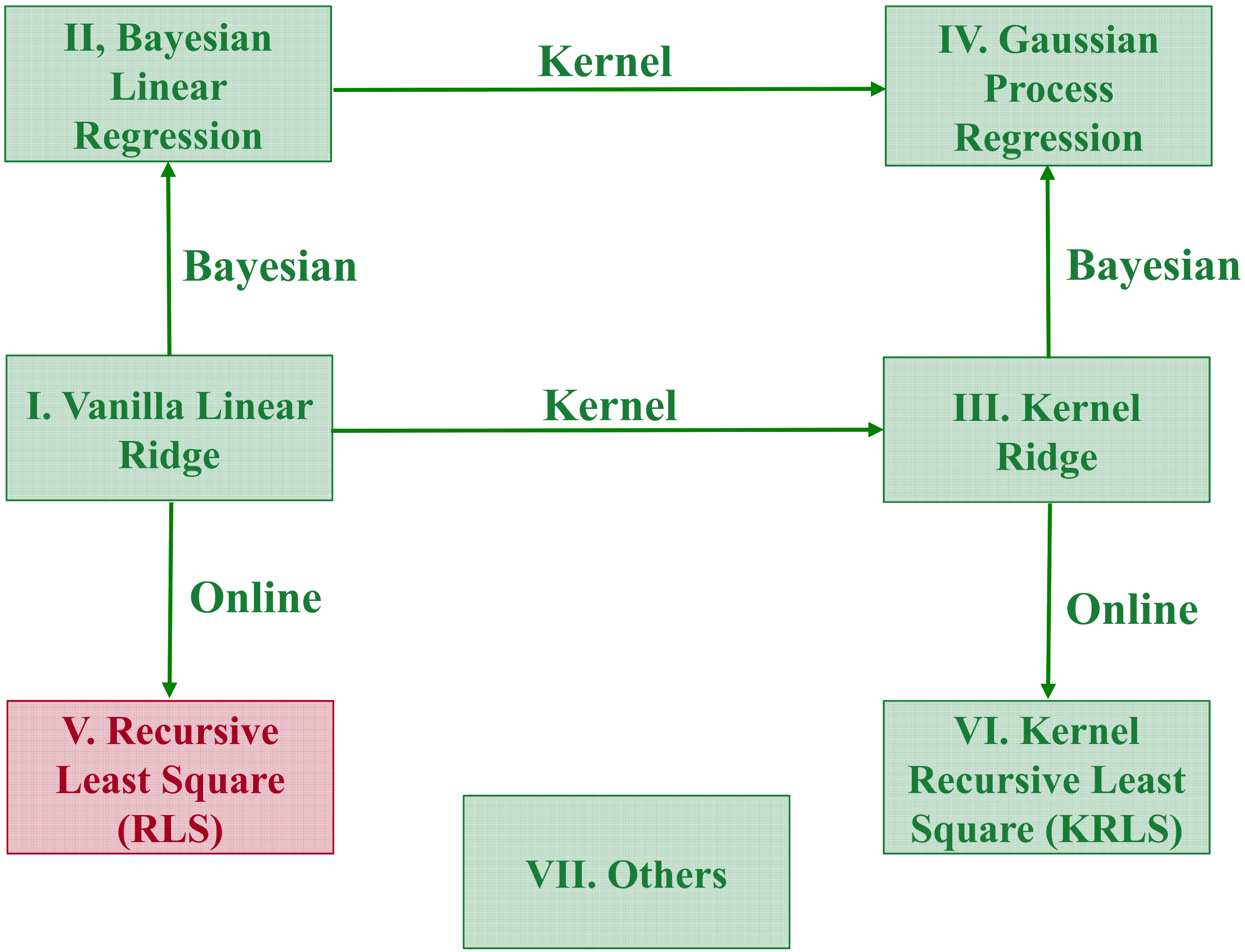

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- **Formalization (1)**

$$Y_N = X_N \cdot w_N + \varepsilon$$

$$w_N = (\underbrace{X_N^T X_N + \lambda I_d}_{S_N})^{-1} X_N^T Y_N$$

$$S_N = X_N^T X_N + \lambda I_d$$

$$S_{N+1} = X_{N+1}^T X_{N+1} + \lambda I_d = [X_N^T \; x_{n+1}^T] \begin{bmatrix} X_N \\ x_{N+1} \end{bmatrix} + \lambda I_d$$

$$\Rightarrow \boxed{S_{N+1} = S_N + x_{N+1}^T x_{N+1}}$$

$$S_N w_N = X_N^T Y_N$$

$$S_{N+1} w_{N+1} = X_{N+1}^T Y_{N+1} = X_N^T Y_N + x_{n+1}^T y_{n+1}$$

$$\Rightarrow w_{N+1} = w_N + S_{N+1}^{-1} x_{n+1}^T (y_{n+1} - x_{n+1} \cdot w_n)$$

• V. Recursive Least Square (RLS)

- **Formalization (2)**

$$e_n = y_{n+1} - x_{n+1} w_n$$

$$S_{N+1} = S_N + x_{N+1}^T x_{N+1}$$

$$w_{N+1} = w_N + \underline{S_{N+1}^{-1}} x_{N+1}^T e_N$$

Can it be better ?

$$\boxed{\begin{array}{l} ① (A+B)^{-1} = A^{-1} - \frac{1}{1+g} A^{-1} B A^{-1} \\ \quad g = \mathrm{trace}(BA^{-1}) \\ ② \text{ trace trick} \\ \quad tr(uvw) = tr(wuv) = tr(vwu) \end{array}}$$

• V. Recursive Least Square (RLS)

- **Computation Optimization**

$$S_{N+1}^{-1} = (S_N + x_{N+1}^T x_{N+1})^{-1}$$

$$= S_N^{-1} - \frac{1}{1+\underline{tr(x_{N+1}^T x_{N+1} S_N^{-1})}} S_N^{-1} x_{N+1}^T \cdot x_{N+1} S_N^{-1}$$

$O(d^3)$ to $O(d^2)$

$$tr(x_{N+1}^T x_{N+1} S_N^{-1}) = tr(x_{N+1} S_N^{-1} x_{N+1}^T)$$

$$= x_{N+1} S_N^{-1} x_{N+1}^T$$ scalar

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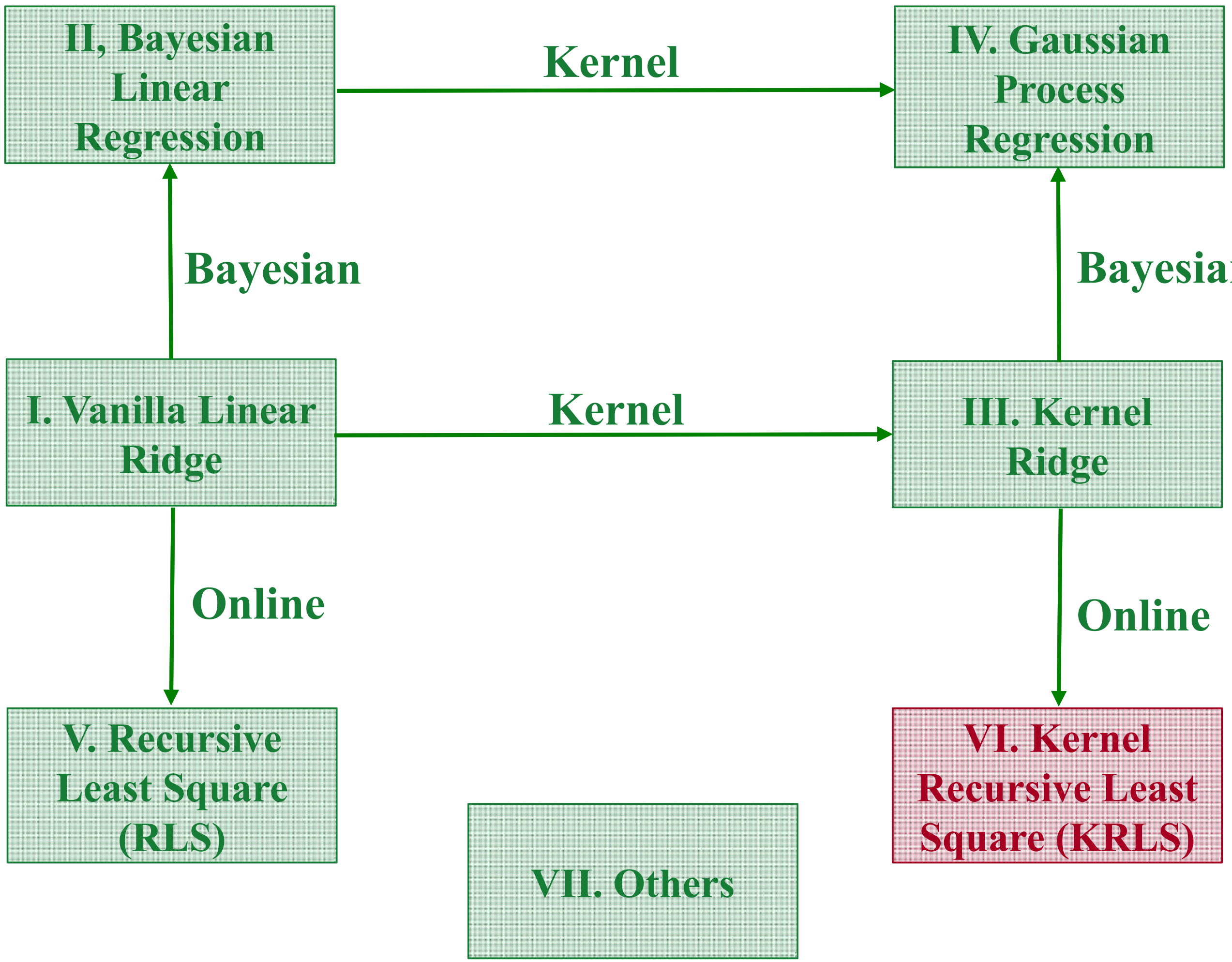
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- **Infinite Dictionary**

- **The core step is to get the inverse of new kernel $O(N^2)$**

$$\dot{\mathbf{K}} = \mathbf{K} + c\mathbf{I} \qquad \dot{\mathbf{K}}_n = \begin{bmatrix} \dot{\mathbf{K}}_{n-1} & \mathbf{k}_n \\ \mathbf{k}_n^\top & k_{nn} + c \end{bmatrix}$$

$$\mathbf{a}_n = \dot{\mathbf{K}}_{n-1}^{-1}\mathbf{k}_n \qquad \gamma_n = k_{nn} + c - \mathbf{k}_n^\top \mathbf{a}_n$$

$$\dot{\mathbf{K}}_n^{-1} = \frac{1}{\gamma_n}\begin{bmatrix} \gamma_n \dot{\mathbf{K}}_{n-1}^{-1} + \mathbf{a}_n \mathbf{a}_n^\top & -\mathbf{a}_n \\ -\mathbf{a}_n & 1 \end{bmatrix}$$

- **The new instance parameters will be easy to get $O(N^2)$**

$$\boldsymbol{\alpha}_{n-1} = \dot{\mathbf{K}}_{n-1}^{-1}\mathbf{y}_{n-1} \qquad \hat{y}_n = \mathbf{k}_n^\top \boldsymbol{\alpha}_{n-1} \qquad e_n = y_n - \hat{y}_n$$

$$\boldsymbol{\alpha}_n = \begin{bmatrix} \boldsymbol{\alpha}_{n-1} - \mathbf{a}_n e_n / \gamma_n \\ e_n / \gamma_n \end{bmatrix}$$

- **There are many criteria for growing and pruning dictionary**

• VI. Kernel Recursive Least Square (KRLS)

- **Dictionary Update**

criterion	type	complexity
all	growing	—
coherence	growing	$\mathcal{O}(m)$
ALD	growing	$\mathcal{O}(m^2)$
oldest	pruning	—
least weight	pruning	$\mathcal{O}(m)$
least a posteriori SE	pruning	$\mathcal{O}(m^2)$

• VI. Kernel Recursive Least Square (KRLS)

- Sliding-Window

- Very simple update to the dictionary: remove the oldest

- Suitable for Time Series

- Inverse Kernel $\dot{\mathrm{K}}_{n-1} = \begin{bmatrix} a & \mathrm{b}^T \\ \mathrm{b} & \mathrm{D} \end{bmatrix}$ $\dot{\mathrm{K}}_{n-1}^{-1} = \begin{bmatrix} e & \mathrm{f}^T \\ \mathrm{f} & \mathrm{G} \end{bmatrix}$

$$\mathrm{D}^{-1} = \mathrm{G} - \mathrm{f}\mathrm{f}^T/e.$$

- Remove the oldest instance, and its instance parameter

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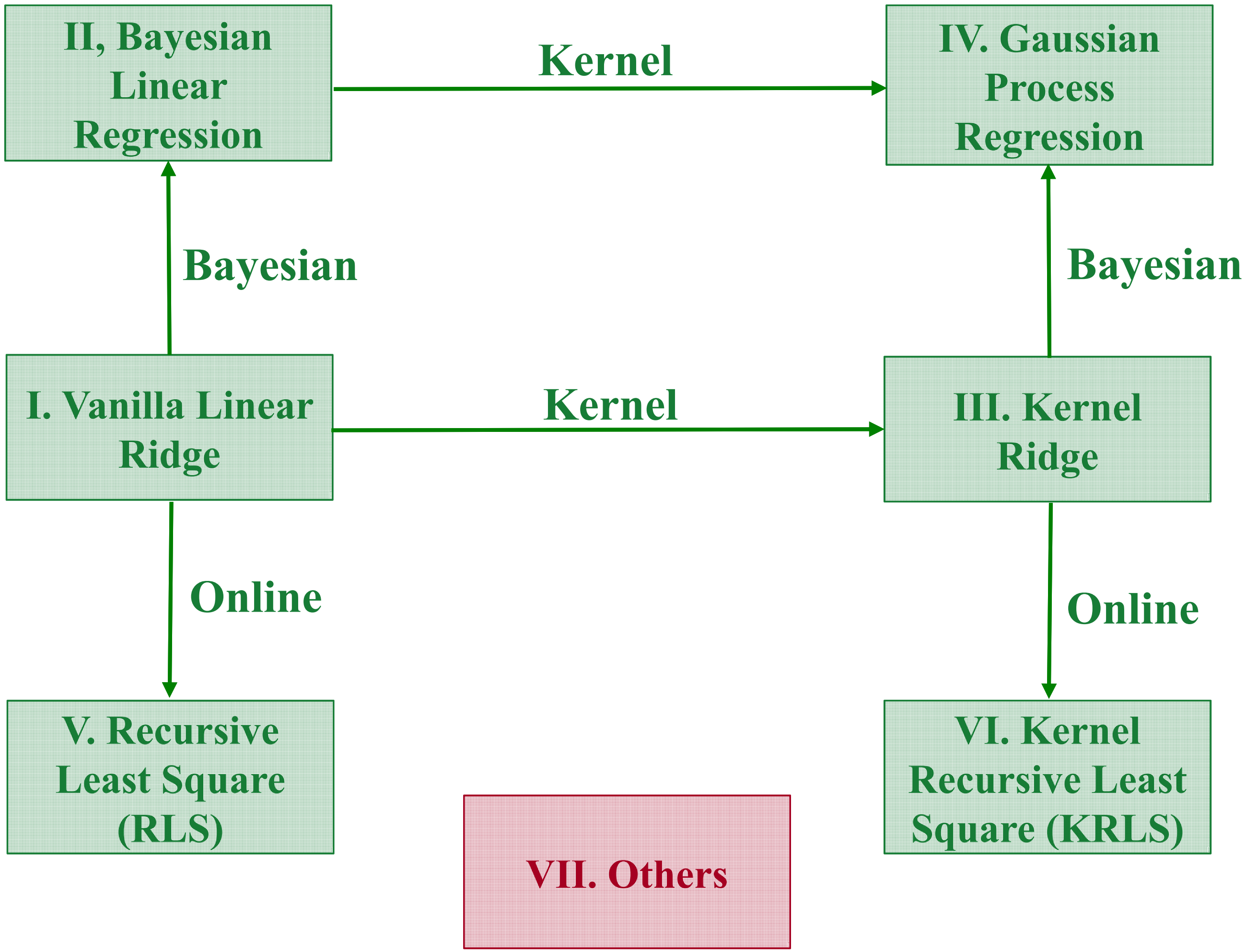

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- **Kalman Filter for Online Linear Regression**

θ_t is the $\boxed{\text{state}}$, y_t is the $\boxed{\text{observation}}$.

$$\begin{cases} \theta_t = a_t \theta_{t-1} + w_t \\ y_t = F_t^T \theta_t + v_t \end{cases}$$

Online linear regression?

$\theta_t \leftarrow \beta_t$, $y_t = \beta_t^T x_t + \varepsilon$

$$\begin{cases} \beta_t = \overbrace{\boxed{I}}^{a_t} \cdot \beta_{t-1} + w_t \\ y_t = \underbrace{\boxed{x_t}}_{F_t^T} \cdot \beta_t + v_t \end{cases}$$

Bibliography

- Online regression with kernel
- Gaussian Processes: A Quick Introduction
- CS229 Lecture note of Gaussian Process
- Bayesian Linear Regression YouTube
- Recursive Least Square (RLS) Otexts
- Dynamic Hedge Ratio Between ETF Pairs Using the Kalman Filter

Thanks for listening!