SPECTRAL METHODS IN GAUSSIAN MODELLING

TOPIC 3: VARIATIONAL INFERENCE

James Requiema and Wessel Bruinsma

University of Cambridge and Invenia Labs

18 January 2019

• RFFs: approximate kernel and perform inference.

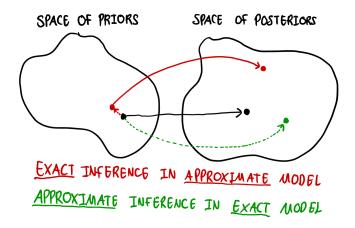
- RFFs: approximate kernel and perform inference.
- \Rightarrow Exact inference in approximate model.

- RFFs: approximate kernel and perform inference.
- \Rightarrow Exact inference in approximate model.
 - Can affect posterior in unforeseen/undesired ways.

- RFFs: approximate kernel and perform inference.
- \Rightarrow Exact inference in approximate model.
 - Can affect posterior in unforeseen/undesired ways.
 - Overfitting

- RFFs: approximate kernel and perform inference.
- ⇒ Exact inference in approximate model.
 - Can affect posterior in unforeseen/undesired ways.
 - Overfitting
 - Should perform approximate inference in exact model.

- RFFs: approximate kernel and perform inference.
- ⇒ Exact inference in approximate model.
 - Can affect posterior in unforeseen/undesired ways.
 - Overfitting
 - Should perform approximate inference in exact model.
 - No overfitting!



• Goal: compute $p(f \mid \mathcal{D})$.

- Goal: compute $p(f | \mathcal{D})$.
- Introduce approximate posterior q(f):

- Goal: compute $p(f | \mathcal{D})$.
- Introduce approximate posterior q(f):

$$\theta^* = \underset{q \in \mathcal{Q}}{\operatorname{arg \, min}} \, \mathrm{D}(q(f) \, \| \, p(f \, | \, \mathcal{D})).$$

- Goal: compute $p(f \mid \mathcal{D})$.
- Introduce approximate posterior q(f):

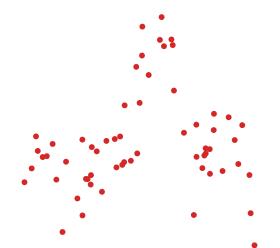
$$\theta^* = \underset{q \in \mathcal{Q}}{\operatorname{arg \, min}} \, \mathrm{D}(q(f) \, \| \, p(f \, | \, \mathcal{D})).$$

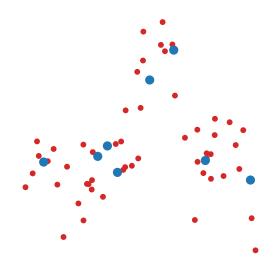
• Often D = KL divergence: variational inference.

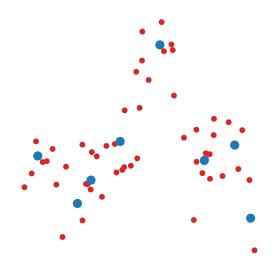
- Goal: compute $p(f | \mathcal{D})$.
- Introduce approximate posterior q(f):

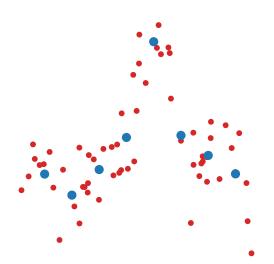
$$\theta^* = \underset{q \in \mathcal{Q}}{\operatorname{arg \, min}} \, \mathrm{D}(q(f) \, \| \, p(f \, | \, \mathcal{D})).$$

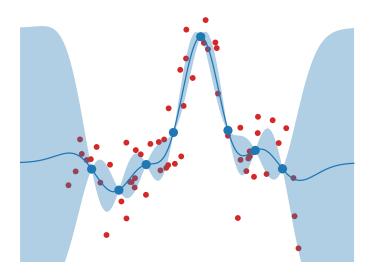
- Often D = KL divergence: variational inference.
- How to construct q(f)?

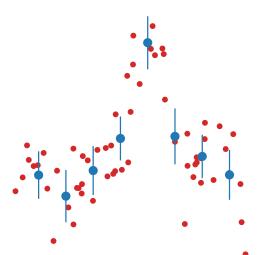


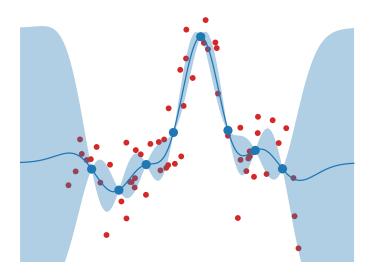


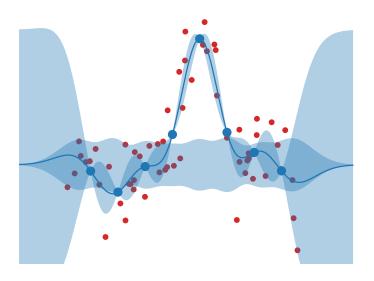


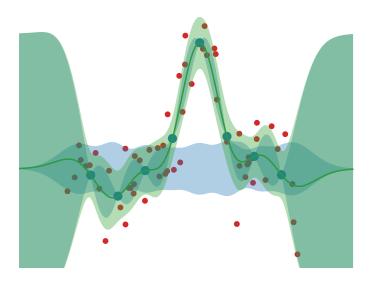












• Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$

- Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$
- Assume distribution q(u).

- Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$
- Assume distribution q(u).
- Inducing point approximation (Titsias, 2009):

$$p(f \mid \mathcal{D}) \approx q(f) \equiv \int p(f \mid u)q(u) du$$

- Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$
- Assume distribution q(u).
- Inducing point approximation (Titsias, 2009):

$$p(f \mid \mathcal{D}) \approx q(f) \equiv \int p(f \mid u)q(u) \, du,$$
$$q^*(u) = \underset{q(u)}{\operatorname{arg \, min}} \, D_{\mathrm{KL}}(q(f) \parallel p(f \mid \mathcal{D}))$$

- Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$
- Assume distribution q(u).
- Inducing point approximation (Titsias, 2009):

$$p(f \mid \mathcal{D}) \approx q(f) \equiv \int p(f \mid u)q(u) \, du,$$

$$q^*(u) = \underset{q(u)}{\operatorname{arg \, min}} \, D_{\mathrm{KL}}(q(f) \parallel p(f \mid \mathcal{D}))$$

$$\propto p(u) \exp \int p(f \mid u) \log p(\mathcal{D} \mid f) \, df.$$

- Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$
- Assume distribution q(u).
- Inducing point approximation (Titsias, 2009):

$$p(f \mid \mathcal{D}) \approx q(f) \equiv \int p(f \mid u)q(u) \, du,$$

$$q^*(u) = \underset{q(u)}{\operatorname{arg \, min}} \, D_{\mathrm{KL}}(q(f) \parallel p(f \mid \mathcal{D}))$$

$$\propto p(u) \exp \int p(f \mid u) \log p(\mathcal{D} \mid f) \, df.$$

• Complexities: Time Memory Full posterior $O(N^3)$ $O(N^2)$ Inducing points

- Introduce inducing points: $u = (f(t_{u,1}), \dots, f(t_{u,M})).$
- Assume distribution q(u).
- Inducing point approximation (Titsias, 2009):

$$p(f \mid \mathcal{D}) \approx q(f) \equiv \int p(f \mid u)q(u) \, du,$$

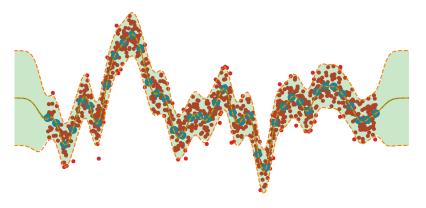
$$q^*(u) = \underset{q(u)}{\operatorname{arg \, min}} \, D_{\mathrm{KL}}(q(f) \parallel p(f \mid \mathcal{D}))$$

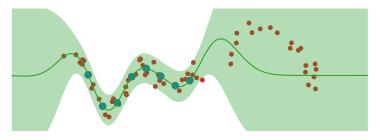
$$\propto p(u) \exp \int p(f \mid u) \log p(\mathcal{D} \mid f) \, df.$$

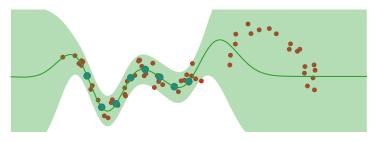
• Complexities: Time Memory Full posterior $O(N^3)$ $O(N^2)$ Inducing points $O(NM^2)$ O(NM)

Example

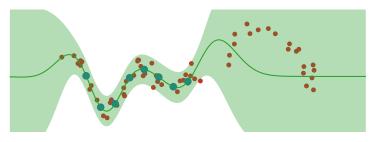
• N = 1000 and M = 40; $25 \times$ compression!



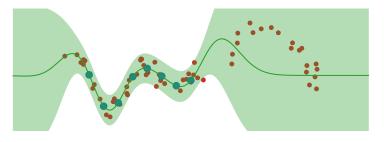




• Need $M \propto N$



• Need $M \propto N$: hidden $O(N^3)$ scaling!



• Need $M \propto N$: hidden $O(N^3)$ scaling!

• SSA: local in spectrum

Inducing points:

+ Appealing approximative construction

- Hidden $O(N^3)$ scaling

SSA:

+ Representative power

Overfitting

Inducing points: SSA: $+ \mbox{ Appealing approximative } + \mbox{ Representative power } \\ \mbox{ construction } - \mbox{ Hidden } O(N^3) \mbox{ scaling } - \mbox{ Overfitting }$

Best of both worlds?

Inducing points:

SSA:

+ Appealing approximative

+ Representative power

construction

- Hidden $O(N^3)$ scaling

Overfitting

Best of both worlds?

Yes: Variational Fourier Features (VFFs)!

(Hensman et al., 2016)

• Extension of inducing point method (Gredilla and Vidal, 2009)

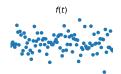
- Extension of inducing point method (Gredilla and Vidal, 2009)
- Introduce pseudo-observations for a linear transform of f:

$$g(\xi) \mid f = \int_{-\infty}^{\infty} h(\xi, t) f(t) dt, \quad u = (g(\xi_{u,1}), \dots, g(\xi_{u,M})).$$

- Extension of inducing point method (Gredilla and Vidal, 2009)
- Introduce pseudo-observations for a linear transform of f:

$$g(\xi) \mid f = \int_{-\infty}^{\infty} h(\xi, t) f(t) dt, \quad u = (g(\xi_{u,1}), \dots, g(\xi_{u,M})).$$

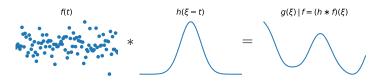
• In some cases, necessary:



- Extension of inducing point method (Gredilla and Vidal, 2009)
- Introduce pseudo-observations for a linear transform of f:

$$g(\xi) \mid f = \int_{-\infty}^{\infty} h(\xi, t) f(t) dt, \quad u = (g(\xi_{u,1}), \dots, g(\xi_{u,M})).$$

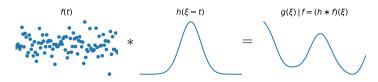
• In some cases, necessary:



- Extension of inducing point method (Gredilla and Vidal, 2009)
- Introduce pseudo-observations for a linear transform of f:

$$g(\xi) \mid f = \int_{-\infty}^{\infty} h(\xi, t) f(t) dt, \quad u = (g(\xi_{u,1}), \dots, g(\xi_{u,M})).$$

• In some cases, necessary:



• In other cases, improve q(f).

• Predictive mean in SSA:

$$\hat{f}^{(SSA)}(t) = \sum_{i=1}^{M} \alpha_i \cos(2\pi \xi_i t) + \sum_{i=1}^{M} \beta_i \sin(2\pi \xi_i t).$$

• Predictive mean in SSA:

$$\hat{f}^{(SSA)}(t) = \sum_{i=1}^{M} \alpha_i \cos(2\pi \xi_i t) + \sum_{i=1}^{M} \beta_i \sin(2\pi \xi_i t).$$

• Predictive mean for inter-domain inducing points:

$$\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i \int_{-\infty}^{\infty} k(t, \tau) h(\xi_{u,i}, \tau) d\tau.$$

• Predictive mean in SSA:

$$\hat{f}^{(\mathrm{SSA})}(t) = \sum_{i=1}^{M} \alpha_i \cos(2\pi \xi_i t) + \sum_{i=1}^{M} \beta_i \sin(2\pi \xi_i t).$$

• Predictive mean for inter-domain inducing points:

$$\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i \int_{-\infty}^{\infty} k(t, \tau) h(\xi_{u,i}, \tau) \, d\tau.$$

• VFFs: engineer h such that $\hat{f}^{(\text{VFF})}$ is also a Fourier expansion.

Attempt 1:
$$g(\xi) \mid f = \int_{-\infty}^{\infty} e^{-2\pi \iota \xi t} f(t) dt$$
.

Attempt 1:
$$g(\xi) \mid f = \int_{-\infty}^{\infty} e^{-2\pi \iota \xi t} f(t) dt$$
.

• Inducing points become inducing frequencies.

Attempt 1:
$$g(\xi) \mid f = \int_{-\infty}^{\infty} e^{-2\pi i \xi t} f(t) dt$$
.

- Inducing points become inducing frequencies.
- $\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i \hat{k}(\xi_{u,i}) e^{-2\pi \iota \xi_{u,i} t}$.

Attempt 1:
$$g(\xi) \mid f = \int_{-\infty}^{\infty} e^{-2\pi \iota \xi t} f(t) dt$$
.

- Inducing points become inducing frequencies.
- $\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i \hat{k}(\xi_{u,i}) e^{-2\pi \iota \xi_{u,i} t}$.
- But g is white noise...

Attempt 1:
$$g(\xi) \mid f = \int_{-\infty}^{\infty} e^{-2\pi i \xi t} f(t) dt$$
.

- Inducing points become inducing frequencies.
- $\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i \hat{k}(\xi_{u,i}) e^{-2\pi \iota \xi_{u,i} t}$.
- But g is white noise...

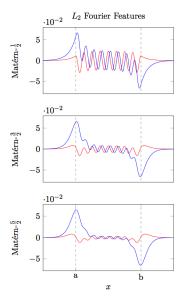
Attempt 2:
$$g(\xi) | f = \int_a^b e^{-2\pi \iota \xi(t-a)} f(t) dt$$
.

Attempt 1:
$$g(\xi) \mid f = \int_{-\infty}^{\infty} e^{-2\pi \iota \xi t} f(t) dt$$
.

- Inducing points become inducing frequencies.
- $\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i \hat{k}(\xi_{u,i}) e^{-2\pi \iota \xi_{u,i} t}$.
- But g is white noise...

Attempt 2:
$$g(\xi) \mid f = \int_a^b e^{-2\pi \iota \xi(t-a)} f(t) dt$$
. $(L^2[a, b]\text{-VFFs})$

• Works, but edge effects near boundaries.



(Figure taken from Hensman et al. (2016).)

• Use tools from RKHS theory to eliminate edge effects.

- Use tools from RKHS theory to eliminate edge effects.
- Mercer's Theorem:

$$k(t,t') = \sum_{i=1}^{\infty} \lambda_i \phi_i(t) \phi_i^*(t')$$

where $(\phi_i)_{i=1}^{\infty}$ and $(\lambda_i)_{i=1}^{\infty}$ e.f.'s and e.v.'s of

$$T_k f = t \mapsto \langle k(t, \cdot), f \rangle, \qquad \langle f, g \rangle = \int_a^b f(t) g^*(t) d\mu(t).$$

- Use tools from RKHS theory to eliminate edge effects.
- Mercer's Theorem:

$$k(t,t') = \sum_{i=1}^{\infty} \lambda_i \phi_i(t) \phi_i^*(t')$$

where $(\phi_i)_{i=1}^{\infty}$ and $(\lambda_i)_{i=1}^{\infty}$ e.f.'s and e.v.'s of

$$T_k f = t \mapsto \langle k(t, \cdot), f \rangle, \qquad \langle f, g \rangle = \int_a^b f(t) g^*(t) d\mu(t).$$

• Why?

- Use tools from RKHS theory to eliminate edge effects.
- Mercer's Theorem:

$$k(t,t') = \sum_{i=1}^{\infty} \lambda_i \phi_i(t) \phi_i^*(t')$$

where $(\phi_i)_{i=1}^{\infty}$ and $(\lambda_i)_{i=1}^{\infty}$ e.f.'s and e.v.'s of

$$T_k f = t \mapsto \langle k(t, \cdot), f \rangle, \qquad \langle f, g \rangle = \int_a^b f(t) g^*(t) d\mu(t).$$

• Why?

$$\hat{f}^{(\text{IDIP})}(t) = \sum_{i=1}^{M} \alpha_i T_k(h(\xi_{u,i}, \cdot))(t).$$

• Desire $T_k(h(\xi, \cdot))(t) = \psi(\xi, t) = e^{-2\pi \iota \xi t}$.

- Desire $T_k(h(\xi, \cdot))(t) = \psi(\xi, t) = e^{-2\pi \iota \xi t}$.
- If $\psi(\xi, \cdot) \in \text{span } \{\phi_i\}_{i=1}^{\infty}$, then

$$\psi(\xi,t) = \sum_{i=1}^{\infty} \phi_i(t) \langle \psi(\xi,\,\cdot\,), \phi_i \rangle.$$

- Desire $T_k(h(\xi, \cdot))(t) = \psi(\xi, t) = e^{-2\pi \iota \xi t}$.
- If $\psi(\xi, \cdot) \in \text{span } \{\phi_i\}_{i=1}^{\infty}$, then

$$\psi(\xi,t) = \sum_{i=1}^{\infty} \phi_i(t) \langle \psi(\xi,\,\cdot\,), \phi_i \rangle.$$

• Solution:

$$h(\xi, t) = \sum_{i=1}^{\infty} \frac{1}{\lambda_i} \phi_i(t) \langle \psi(\xi, \cdot), \phi_i \rangle$$

- Desire $T_k(h(\xi, \cdot))(t) = \psi(\xi, t) = e^{-2\pi \iota \xi t}$.
- If $\psi(\xi, \cdot) \in \text{span } \{\phi_i\}_{i=1}^{\infty}$, then

$$\psi(\xi,t) = \sum_{i=1}^{\infty} \phi_i(t) \langle \psi(\xi,\,\cdot\,), \phi_i \rangle.$$

• Solution:

$$h(\xi,t) = \sum_{i=1}^{\infty} \frac{1}{\lambda_i} \phi_i(t) \langle \psi(\xi,\cdot), \phi_i \rangle$$

$$\implies T_k(h(\xi,\cdot))(t) = \sum_{i=1}^{\infty} \frac{1}{\lambda_i} T_k(\phi_i)(t) \langle \psi(\xi,\cdot), \phi_i \rangle$$

- Desire $T_k(h(\xi, \cdot))(t) = \psi(\xi, t) = e^{-2\pi \iota \xi t}$.
- If $\psi(\xi, \cdot) \in \text{span } \{\phi_i\}_{i=1}^{\infty}$, then

$$\psi(\xi,t) = \sum_{i=1}^{\infty} \phi_i(t) \langle \psi(\xi,\,\cdot\,), \phi_i \rangle.$$

• Solution:

$$h(\xi,t) = \sum_{i=1}^{\infty} \frac{1}{\lambda_i} \phi_i(t) \langle \psi(\xi, \cdot), \phi_i \rangle$$

$$\implies T_k(h(\xi, \cdot))(t) = \sum_{i=1}^{\infty} \frac{1}{\lambda_i} T_k(\phi_i)(t) \langle \psi(\xi, \cdot), \phi_i \rangle$$

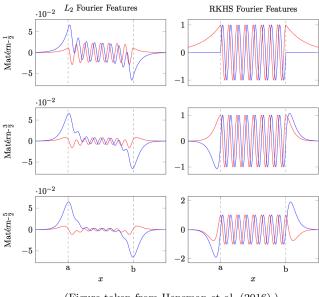
$$= \sum_{i=1}^{\infty} \phi_i(t) \langle \psi(\xi, \cdot), \phi_i \rangle = \psi(\xi, t).$$

• Works for Matérn kernels of half-integer order!

 $\Rightarrow VFFs$

(RKHS-VFFs)

Variational Fourier Features (7)



(Figure taken from Hensman et al. (2016).)

• RFFs simple: amenable to convergence analysis.

- RFFs simple: amenable to convergence analysis.
- Inducing points more complex: convergence analysis hard.

- RFFs simple: amenable to convergence analysis.
- Inducing points more complex: convergence analysis hard.
- Recent result by Burt et al. (2018):

Theorem

Fix $\varepsilon > 0$ and $\delta > 0$. Let $(t_i)_{i=1}^{\infty}$ be sampled i.i.d. from $\mathcal{N}(0, \alpha)$, let k be an exponentiated-quadratic kernel, and let μ have density $\mathcal{N}(0,\beta)$ with $\beta > 2\alpha$. Then there are \tilde{N} and \tilde{C} such that, for all $N > \tilde{N}$, the inter-domain point method with $M = \tilde{C} \log N$ eigenfunction inducing features achieves $D_{\mathrm{KL}}(q(f) \parallel p(f \mid \mathcal{D})) \leq \varepsilon$ with probability at least $1 - \delta$.

Eigenfunction Inducing Features

• Eigenfunction inducing features:

$$u_i \mid f = \frac{1}{\sqrt{\lambda_i}} \int f(t)\phi_i(t) d\mu(t).$$

Eigenfunction Inducing Features

• Eigenfunction inducing features:

$$u_i \mid f = \frac{1}{\sqrt{\lambda_i}} \int f(t)\phi_i(t) d\mu(t).$$

• Nice behaviour:

$$\mathbb{E}[u_i u_j] = 1 \text{ if } i = j \text{ else } 0, \qquad \mathbb{E}[f(t_i)u_j] = \sqrt{\lambda_j}\phi_j(t_i).$$

Eigenfunction Inducing Features

• Eigenfunction inducing features:

$$u_i \mid f = \frac{1}{\sqrt{\lambda_i}} \int f(t)\phi_i(t) d\mu(t).$$

• Nice behaviour:

$$\mathbb{E}[u_i u_j] = 1 \text{ if } i = j \text{ else } 0, \qquad \mathbb{E}[f(t_i) u_j] = \sqrt{\lambda_j} \phi_j(t_i).$$

• Key quantity:

$$c = \operatorname{tr}(K_{ff} - K_{fu}K_{uu}^{-1}K_{fu}),$$

$$(K_{ff})_{ij} = \mathbb{E}[f(t_i)f(t_j)], \qquad (K_{fu})_{ij} = \mathbb{E}[f(t_i)u_j],$$

$$(K_{uu})_{ij} = \mathbb{E}[u_iu_j].$$

Sketch of Proof

• Can compute e.f.'s and e.v.'s for EQ kernel.

Sketch of Proof

- Can compute e.f.'s and e.v.'s for EQ kernel.
- Key inequality:

$$D_{KL}(q(f) || p(f | D)) \le \frac{c}{2\sigma^2} \left(1 + \frac{||y||^2}{\sigma^2 + c}\right).$$

Sketch of Proof

- Can compute e.f.'s and e.v.'s for EQ kernel.
- Key inequality:

$$D_{KL}(q(f) || p(f | D)) \le \frac{c}{2\sigma^2} \left(1 + \frac{||y||^2}{\sigma^2 + c}\right).$$

Bound follows from application of Chebyshev's to

$$\frac{1}{N}c = \sum_{m=M+1}^{\infty} \lambda_m \left[\frac{1}{N} \sum_{i=1}^{N} \phi_m^2(t_i) \right]$$

combined with $\sum_{m=M+1}^{\infty} \lambda_m = O(A^M)$ for some $A \in (0,1)$.

• RFFs: exact inference in approximate model.

• RFFs: exact inference in approximate model.

+ Good representative power

- RFFs: exact inference in approximate model.
 - + Good representative power
- Inducing points: approximate inference in exact model.

- RFFs: exact inference in approximate model.
 - + Good representative power
- Inducing points: approximate inference in exact model.
 - + No overfitting

- RFFs: exact inference in approximate model.
 - + Good representative power
- Inducing points: approximate inference in exact model.
 - + No overfitting
- VFFs = inducing points + representative power of RFFs.

- RFFs: exact inference in approximate model.
 - + Good representative power
- Inducing points: approximate inference in exact model.
 - + No overfitting
- VFFs = inducing points + representative power of RFFs.
- Can design inducing point methods amenable to convergence analysis.