Low Rank Gaussian Processes

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Outline

Parametric Bottleneck

Nonparametric Gaussian Processes

- This work takes us from parametric to non-parametric.
- The limit implies infinite dimensional $\mathbf{w}$.
- Gaussian processes are generally non-parametric: combine data with covariance function to get model.
- This representation *cannot* be summarized by a parameter vector of a fixed size.

The Parametric Bottleneck

- Parametric models have a representation that does not respond to increasing training set size.
- Bayesian posterior distributions over parameters contain the information about the training data.
  - Use Bayes' rule from training data, $p(\mathbf{w}|\mathbf{y}, \mathbf{X})$,
  - Make predictions on test data

$$p(y_*|\mathbf{X}_*, \mathbf{y}, \mathbf{X}) = \int p(y_*|\mathbf{w}, \mathbf{X}_*)\, p(\mathbf{w}|\mathbf{y}, \mathbf{X})\mathrm{d}\mathbf{w}) .$$

- $\mathbf{w}$ becomes a bottleneck for information about the training set to pass to the test set.
- Solution: increase m so that the bottleneck is so large that it no longer presents a problem.
- How big is big enough for m? Non-parametrics says $m \to \infty$.

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- These are known as degenerate covariance matrices.
- Their rank is at most m, non-parametric models have full rank covariance matrices.
- Most well known is the "linear kernel", $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$.

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- Parametric is a special case when conditional prediction can be summarized in a *fixed* number of parameters.
- Complexity of parametric model remains fixed regardless of the size of our training data set.
- For a non-parametric model the required number of parameters grows with the size of the training data.

Low Rank Motivation

Inference in a GP has the following demands:

$$\begin{aligned}\text{Complexity:} \quad & \mathcal{O}(n^3) \\ \text{Storage:} \quad & \mathcal{O}(n^2)\end{aligned}$$

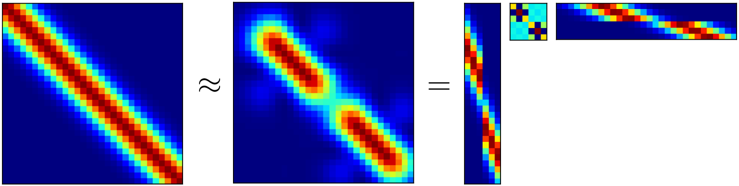
Inference in a low rank GP has the following demands:

$$\begin{aligned}\text{Complexity:} \quad & \mathcal{O}(nm^2) \\ \text{Storage:} \quad & \mathcal{O}(nm)\end{aligned}$$

where m is a user chosen parameter.

Computational Savings

(Smola and Bartlett, 2001; Csató and Opper, 2001, 2002; Csató, 2002; Seeger et al., 2003)

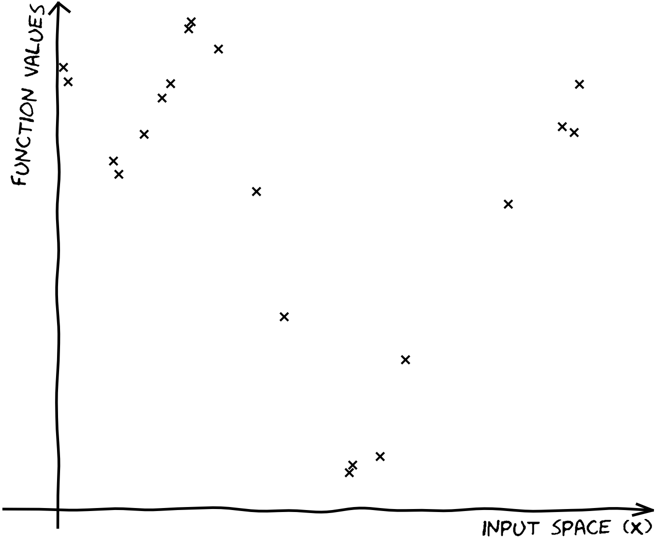


$$\mathbf{K_{ff}} \approx \mathbf{Q_{ff}} = \mathbf{K_{fu}} \mathbf{K_{uu}^{-1}} \mathbf{K_{uf}}$$

Instead of inverting $\mathbf{K_{ff}}$, we make a low rank (or Nyström) approximation, and invert $\mathbf{K_{uu}}$ instead.

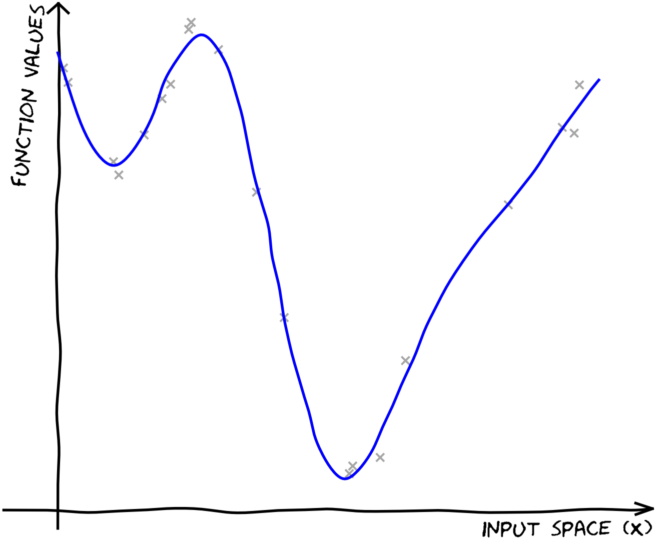
Figure originally from presentation by Ed Snelson at NIPS

$\mathbf{X}, \mathbf{y}$



$\mathbf{X}, \mathbf{y}$

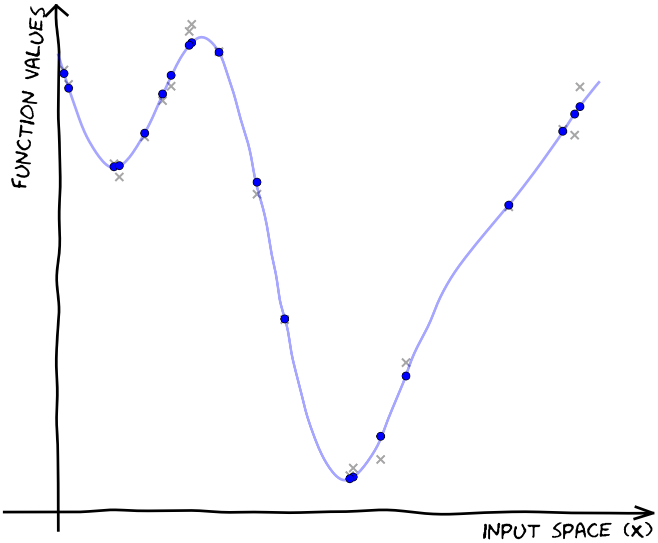
$f(\mathbf{x}) \sim \mathcal{GP}$



$\mathbf{X}, \mathbf{y}$

$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathbf{ff}})$



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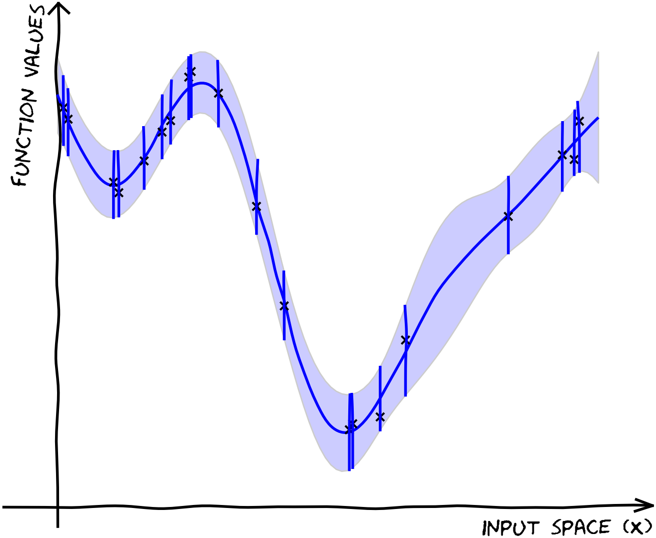
$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$



Introducing $\mathbf{u}$

Take an extra m points on the function, $\mathbf{u} = f(\mathbf{Z})$.

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}) p(\mathbf{u})$$

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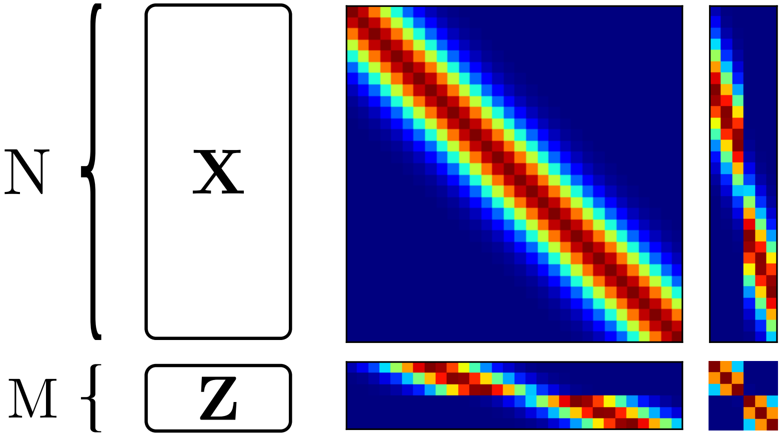

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Take and extra M points on the function, $\mathbf{u} = f(\mathbf{Z})$.

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y} \,|\, \mathbf{f}) p(\mathbf{f} \,|\, \mathbf{u}) p(\mathbf{u})$$

$$\begin{aligned} p(\mathbf{y} \,|\, \mathbf{f}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{f}, \sigma^2 \mathbf{I}\right) \\ p(\mathbf{f} \,|\, \mathbf{u}) &= \mathcal{N}\left(\mathbf{f}|\mathbf{K}_{\mathbf{fu}}\mathbf{K}_{\mathbf{uu}}^{-1}\mathbf{u}, \widetilde{\mathbf{K}}\right) \\ p(\mathbf{u}) &= \mathcal{N}\left(\mathbf{u}|\mathbf{0}, \mathbf{K}_{\mathbf{uu}}\right) \end{aligned}$$

$\mathbf{X}, \mathbf{y}$

$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathbf{ff}})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

$\mathbf{Z}, \mathbf{u}$

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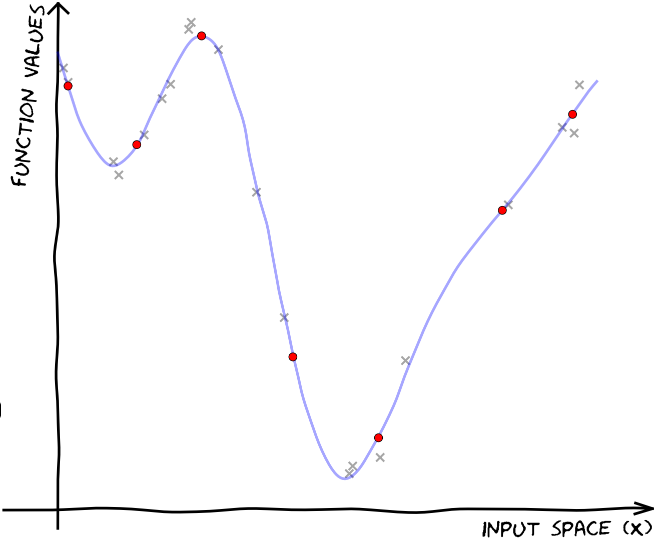

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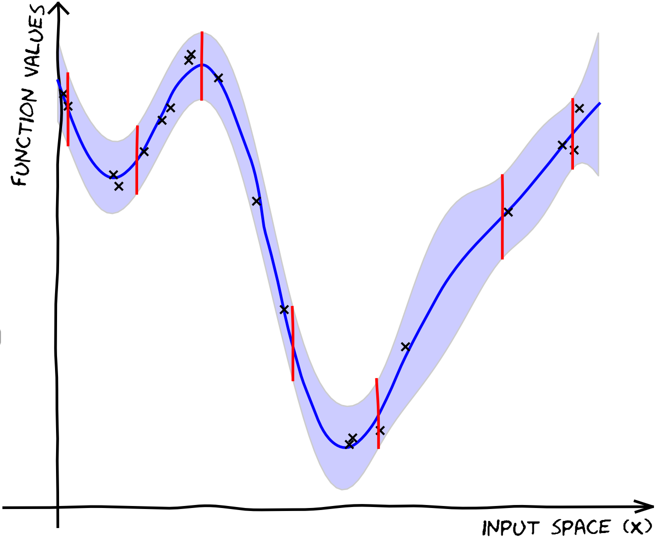
$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

$p(\mathbf{u}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{\mathbf{uu}})$

$\widetilde{p}(\mathbf{u} \mid \mathbf{y}, \mathbf{X})$



The alternative posterior

Instead of doing

$$p(\mathbf{f}|\mathbf{y},\mathbf{X}) = \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{X})}{\int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{X})\mathrm{d}\mathbf{f}}$$

We'll do

$$p(\mathbf{u}|\mathbf{y},\mathbf{Z}) = \frac{p(\mathbf{y}|\mathbf{u})p(\mathbf{u}|\mathbf{Z})}{\int p(\mathbf{y}|\mathbf{u})p(\mathbf{u}|\mathbf{Z})\mathrm{d}\mathbf{u}}$$

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but $p(\mathbf{y}\,|\,\mathbf{u})$ involves inverting $\mathbf{K}_{\mathbf{ff}}$

Variational marginalisation of $\mathbf{f}$

$$\log p(\mathbf{y}|\mathbf{u}) = \log \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u},\mathbf{X})\mathrm{d}\mathbf{f}$$

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$$\log p(\mathbf{y}\,|\,\mathbf{u}) = \log \mathbb{E}_{p(\mathbf{f}\,|\,\mathbf{u},\mathbf{X})}\left[p(\mathbf{y}\,|\,\mathbf{f})\right]$$

Variational marginalisation of $\mathbf{f}$

$$\log p(\mathbf{y} \mid \mathbf{u}) = \log \int p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}) \mathrm{d}\mathbf{f}$$

$$\log p(\mathbf{y} \mid \mathbf{u}) = \log \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X})} \left[p(\mathbf{y} \mid \mathbf{f}) \right]$$

$$\log p(\mathbf{y} \mid \mathbf{u}) \geq \mathbb{E}_{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X})} \left[\log p(\mathbf{y} \mid \mathbf{f}) \right] \triangleq \log \widetilde{p}(\mathbf{y} \mid \mathbf{u})$$

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No inversion of $\mathbf{K}_{\mathbf{ff}}$ required

Variational marginalisation of $\mathbf{f}$ (another way)

(Titsias, 2009)

$$p(\mathbf{y} \,|\, \mathbf{u}) = \frac{p(\mathbf{y} \,|\, \mathbf{f})p(\mathbf{f} \,|\, \mathbf{u})}{p(\mathbf{f} \,|\, \mathbf{y}, \mathbf{u})}$$

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$$\log p(\mathbf{y}\,|\,\mathbf{u}) = \log p(\mathbf{y}\,|\,\mathbf{f}) + \log \frac{p(\mathbf{f}\,|\,\mathbf{u})}{p(\mathbf{f}\,|\,\mathbf{y},\mathbf{u})}$$

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$$\log p(\mathbf{y}\,|\,\mathbf{u}) = \widetilde{p}(\mathbf{y}\,|\,\mathbf{u}) + \mathrm{KL}[p(\mathbf{f}|\mathbf{u})||p(\mathbf{f}\,|\,\mathbf{y},\mathbf{u})]$$

No inversion of $\mathbf{K}_{\mathbf{ff}}$ required

A Lower Bound on the Likelihood

$$\widetilde{p}(\mathbf{y}\,|\,\mathbf{u}) = \prod_{i=1}^{n} \widetilde{p}(y_i\,|\,\mathbf{u})$$

$$\widetilde{p}(y\,|\,\mathbf{u}) = \mathcal{N}\left(y|\mathbf{k}_{f\mathbf{u}}\mathbf{K}_{\mathbf{uu}}^{-1}\mathbf{u}, \sigma^2\right) \exp\left\{-\frac{1}{2\sigma^2}\left(k_{ff} - \mathbf{k}_{f\mathbf{u}}\mathbf{K}_{\mathbf{uu}}^{-1}\mathbf{k}_{\mathbf{u}f}\right)\right\}$$

A straightforward likelihood approximation, and a penalty term

Now we can marginalise $\mathbf{u}$

$$\widetilde{p}(\mathbf{u} \,|\, \mathbf{y}, \mathbf{Z}) = \frac{\widetilde{p}(\mathbf{y} \,|\, \mathbf{u}) p(\mathbf{u} \,|\, \mathbf{Z})}{\int \widetilde{p}(\mathbf{y} \,|\, \mathbf{u}) p(\mathbf{u} \,|\, \mathbf{Z}) \mathrm{d}\mathbf{u}}$$

- Computing the posterior costs $\mathcal{O}(nm^2)$
- We also get a lower bound of the marginal likelihood

What does the penalty term do?

$$\sum_{i=1}^{n} -\frac{1}{2\sigma^2}\left(k_{ff} - \mathbf{k}_{f\mathbf{u}}\mathbf{K}_{\mathbf{uu}}^{-1}\mathbf{k}_{\mathbf{u}f}\right)$$

It doesn't affect the posterior

It appears on the top and bottom of Bayes' rule

$$\widetilde{p}(\mathbf{u}\,|\,\mathbf{y},\mathbf{Z}) = \frac{\widetilde{p}(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})}{\int \widetilde{p}(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})\mathrm{d}\mathbf{u}}$$

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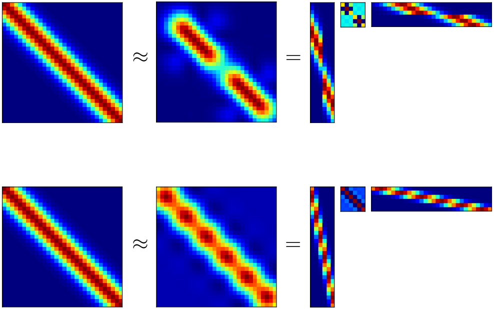

How good is the inducing approximation?

It's easy to show that as $\mathbf{Z} \to \mathbf{X}$:

- $\mathbf{u} \to \mathbf{f}$ (and the posterior is exact)
- The penalty term is zero.
- The cost returns to $\mathcal{O}(n^3)$

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- We're okay if we have sufficient coverage with $\mathbf{Z}$
- We can optimize $\mathbf{Z}$ along with the hyperparameters

Predictions

In a 'full' GP, we did

$$p(f_\star \mid \mathbf{y}) = \int p(f_\star \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{y}) \mathrm{d}\mathbf{f}$$

In a induced GP, we do

$$p(f_\star \mid \mathbf{y}) = \int p(f_\star \mid \mathbf{u}) \widetilde{p}(\mathbf{u} \mid \mathbf{y}) \mathrm{d}\mathbf{u}$$

Recap

So far we:

- introduced $\mathbf{Z}, \mathbf{u}$
- approximated the intergral over $\mathbf{f}$ variationally
- captured the information in $\widetilde{p}(\mathbf{u} \,|\, \mathbf{y})$
- obtained a lower bound on the marginal likeihood
- saw the effect of the penalty term
- prediction for new points

Omitted details:

- optimization of the covariance parameters using the bound
- optimization of Z (simultaneously)
- the form of $\widetilde{p}(\mathbf{u} \,|\, \mathbf{y})$
- historical approximations

Other approximations

Subset selection (Lawrence et al., 2003)

- Random or systematic
- Set $\mathbf{Z}$ to subset of $\mathbf{X}$
- Set $\mathbf{u}$ to subset of $\mathbf{f}$
- Approximation to $p(\mathbf{y}|\mathbf{u})$:
  - $p(\mathbf{y}_i|\mathbf{u}) = p(\mathbf{y}_i|\mathbf{f}_i) \qquad i \in \text{selection}$
  - $p(\mathbf{y}_i|\mathbf{u}) = 1 \qquad i \notin \text{selection}$

Other approximations

(Quiñonero Candela and Rasmussen, 2005) Deterministic Training Conditional (DTC)

- Approximation to $p(\mathbf{y} \mid \mathbf{u})$:
  - $\widetilde{p}(\mathbf{y}_i \mid \mathbf{u}) = \delta(\mathbf{y}_i, \mathbb{E}[\mathbf{f}_i \mid \mathbf{u}])$
- As our variational formulation, but without penalty

Optimization of $\mathbf{Z}$ is difficult

Other approximations

Fully Independent Training Conditional (Snelson and Ghahramani, 2006)

- Approximation to $p(\mathbf{y} \mid \mathbf{u})$:
- $p(\mathbf{y} \mid \mathbf{u}) = \prod_i p(\mathbf{y}_i \mid \mathbf{u})$

Optimization of $\mathbf{Z}$ is still difficult, and there are some weird heteroscedatic effects

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