Using Gaussian Processes: Models, Applications, and Connections

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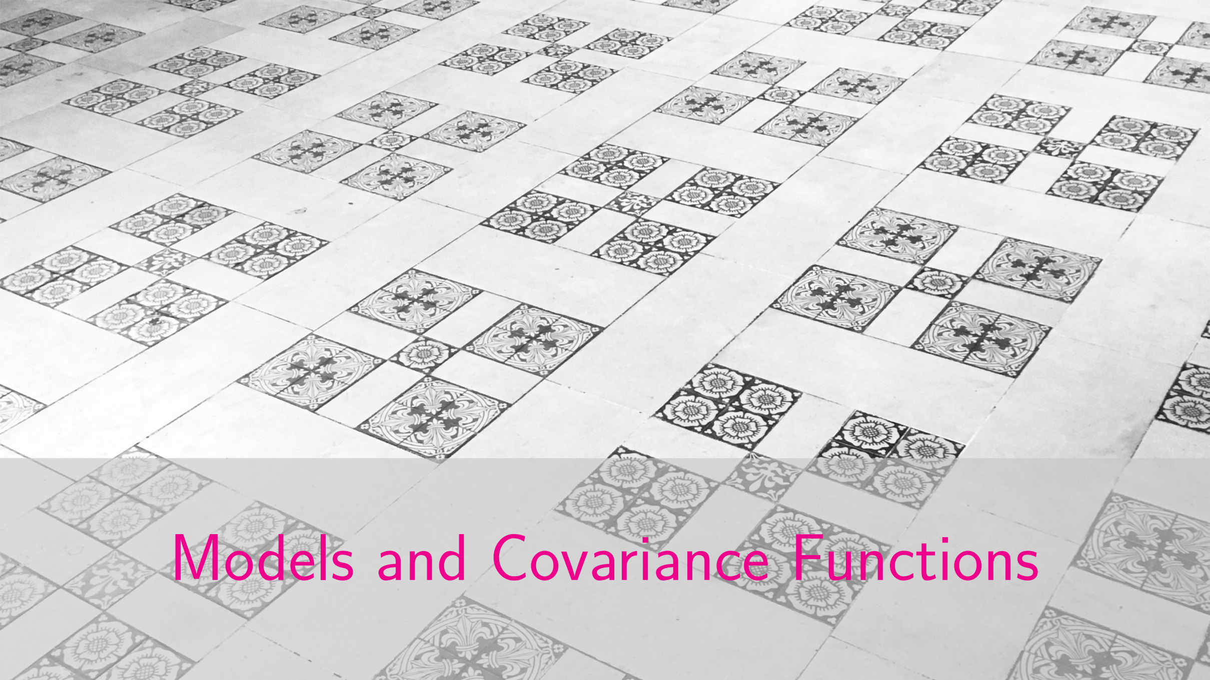
Outline of the tutorial

- **An Introduction to GPs**
  - Mathematical foundations
  - Hyper-parameter learning
  - Covariance functions
  - Multi-dimensional inputs
- **Using GPs: Models, Applications and Connections**
  - Models and more on covariance functions
  - Applications
  - Connections
- **GPs for large data and non-linear models**
  - Scaling through pseudo-data
  - Variational Inference
  - General Approximate inference



Models and Covariance Functions

Big fat covariance function quiz

Which are GPs? Compute the GPs mean and covariance functions.

1. Addition of two GPs

$$f(x) = f_1(x) + f_2(x)$$

$$f_1(x) \sim \mathcal{GP}(0, \Sigma_1(x, x'))$$
$$f_2(x) \sim \mathcal{GP}(0, \Sigma_2(x, x'))$$

2. Random linear model

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More generally: GPs closed under linear transformation / combination:

GP multiplied by a deterministic function = GP,
derivatives of GP = GP, integral of a GP = GP,
convolution of a GP by a deterministic function = GP

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GPs encompass Bayesian linear regression
Not all GPs are non-parametric (infinite numbers of parameters)

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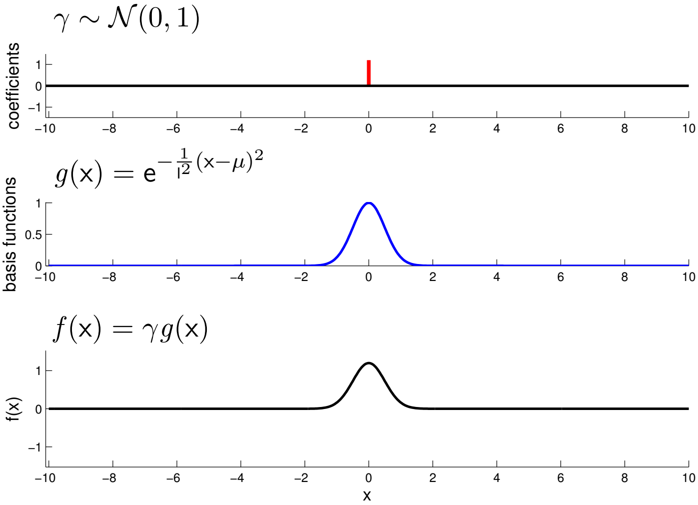
Bochner's theorem: Any stationary covariance function can be written as:

$$\Sigma(x - x') = \int \sigma^2(\omega) \cos(\omega(x - x'))\mathrm{d}\omega$$

roughly, the function comprises "an uncountably infinite sum of random sins and cosines"

Basis function view of Gaussian processes



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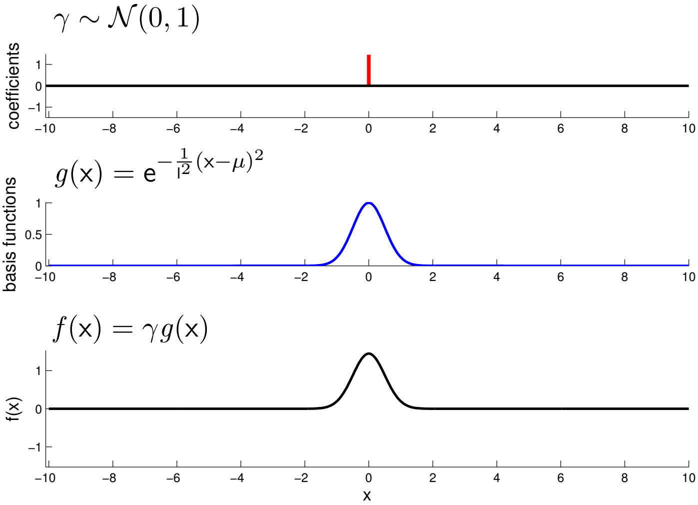

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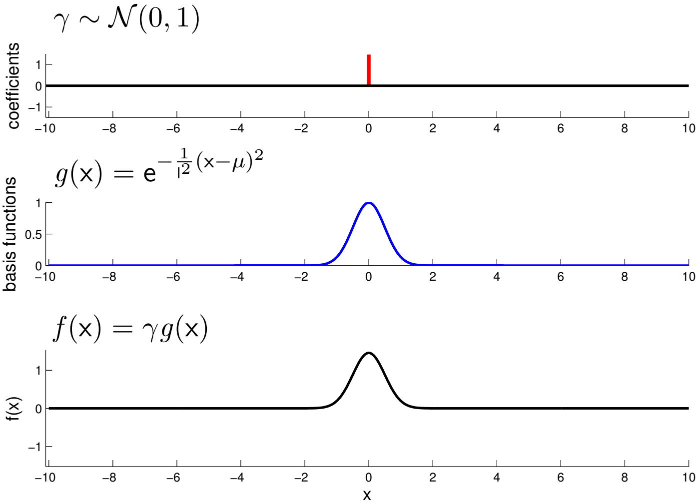

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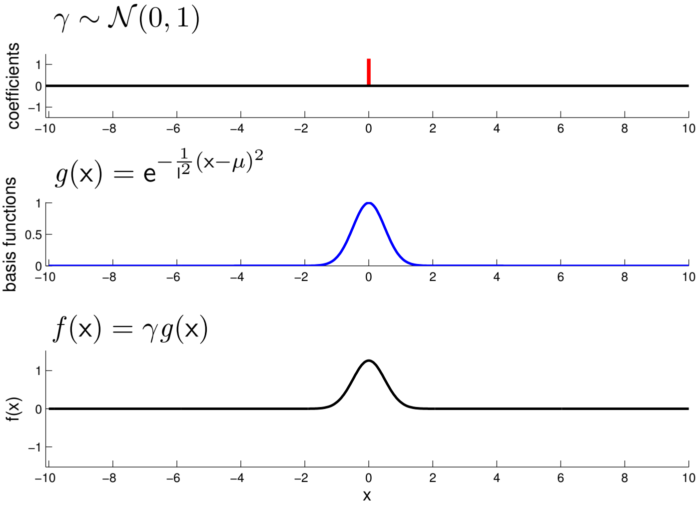

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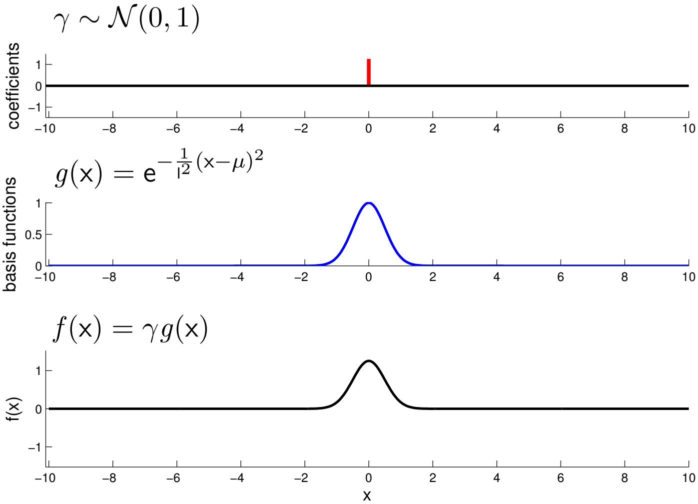

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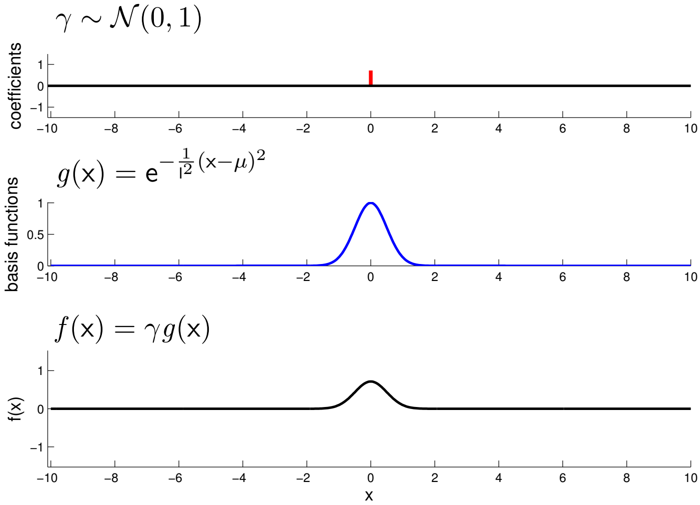

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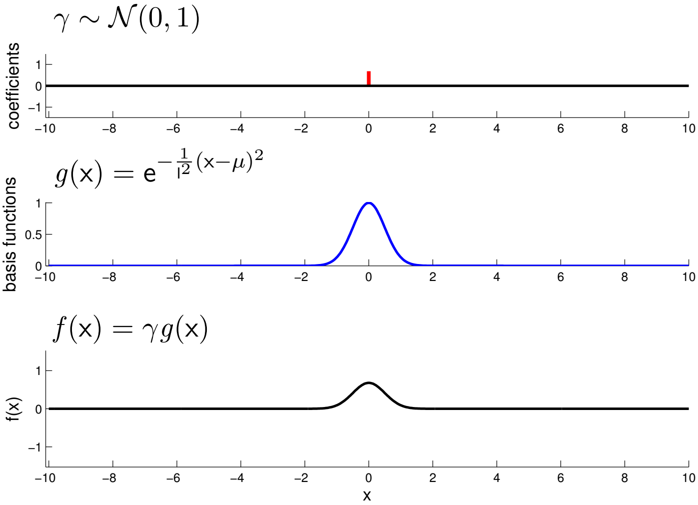

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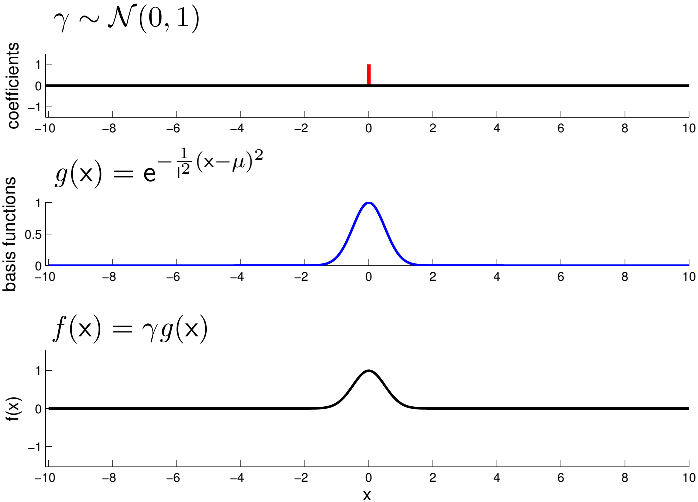

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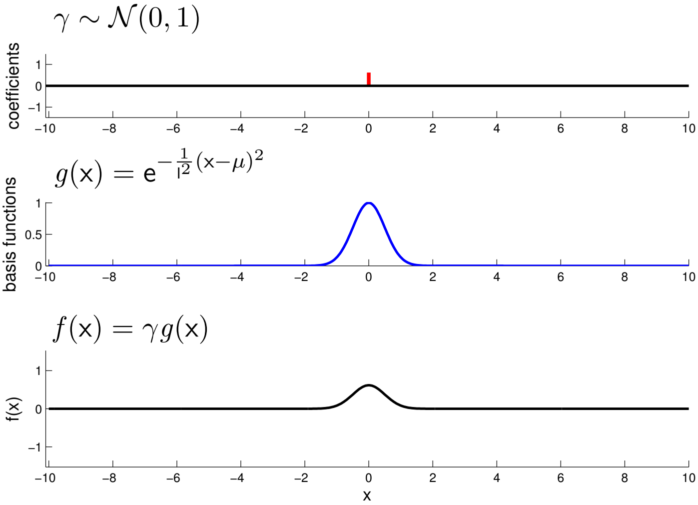

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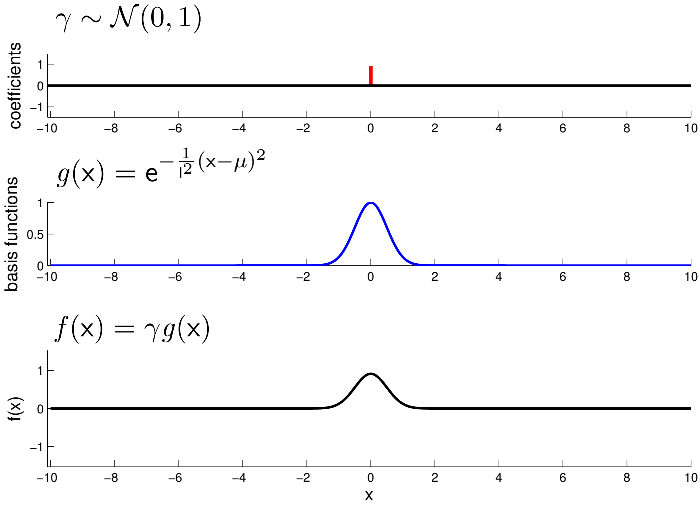

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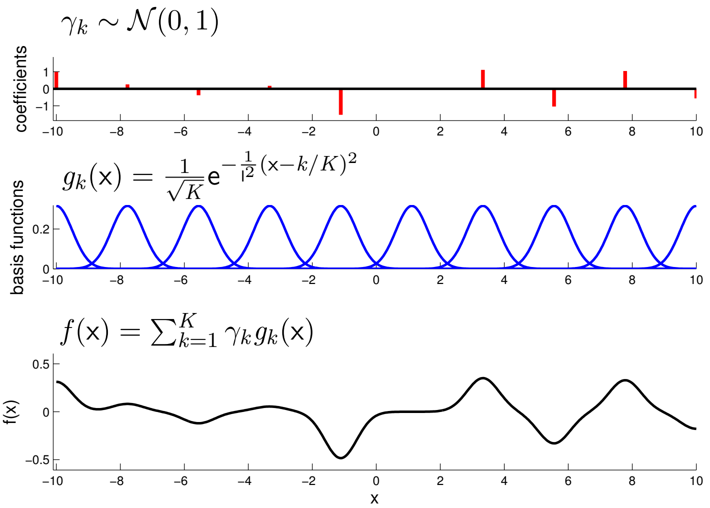

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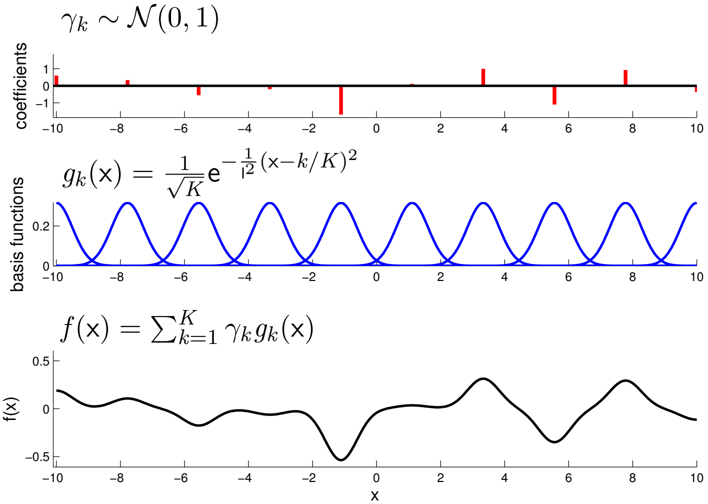

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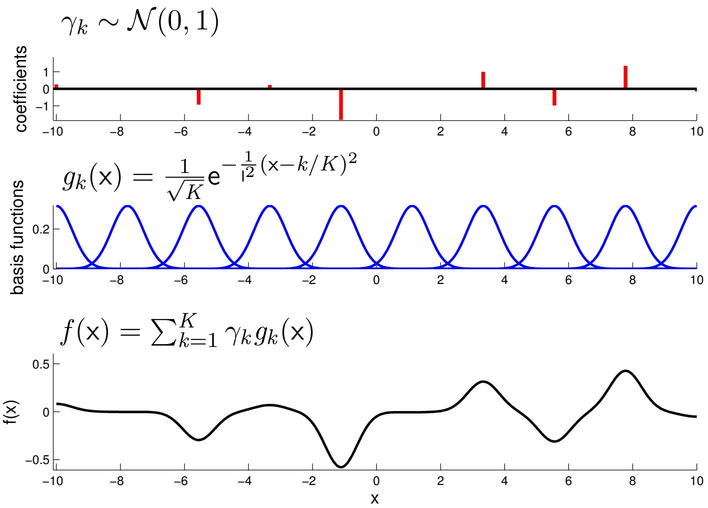

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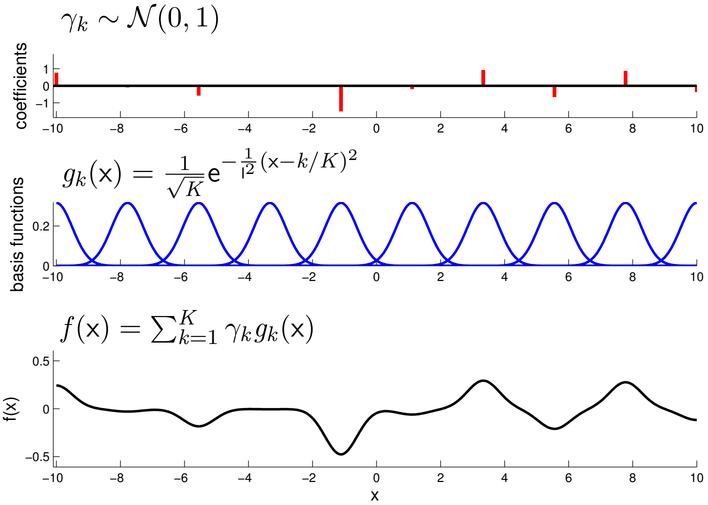

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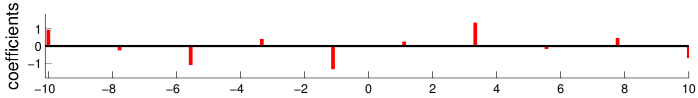
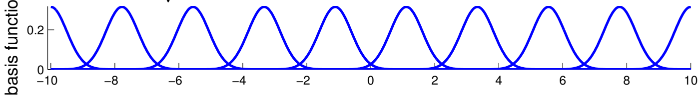
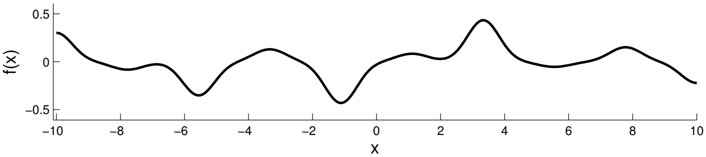
$$\gamma_k \sim \mathcal{N}(0,1)$$



$$g_k(\mathsf{x}) = \frac{1}{\sqrt{K}} \mathsf{e}^{-\frac{1}{\mathsf{l}^2}(\mathsf{x}-k/K)^2}$$



$$f(\mathsf{x}) = \sum_{k=1}^{K} \gamma_k g_k(\mathsf{x})$$



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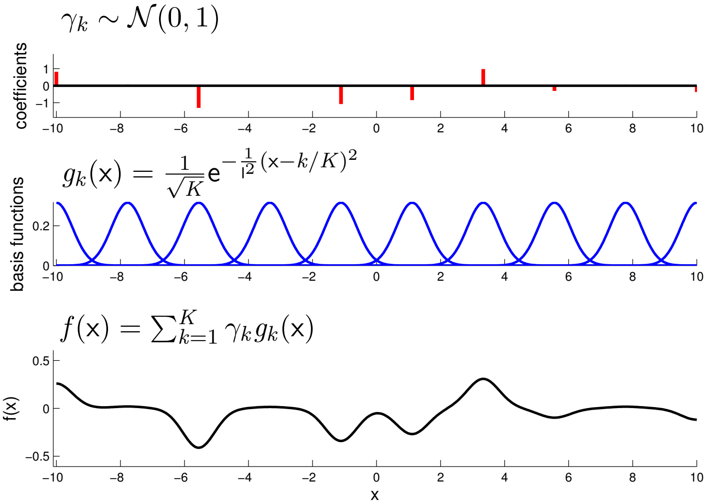

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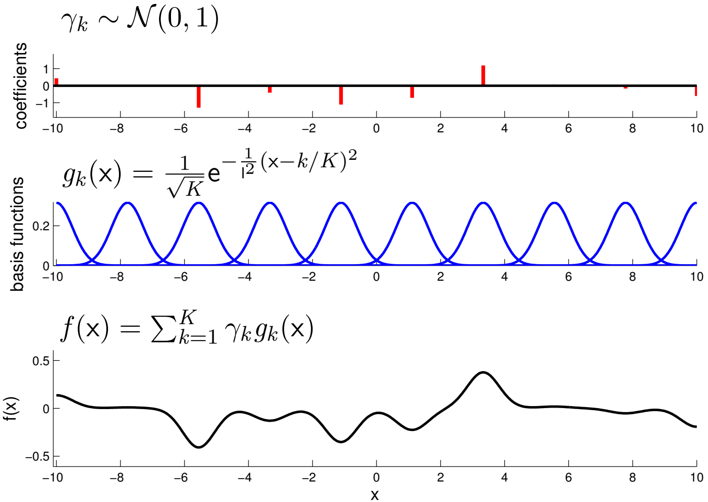

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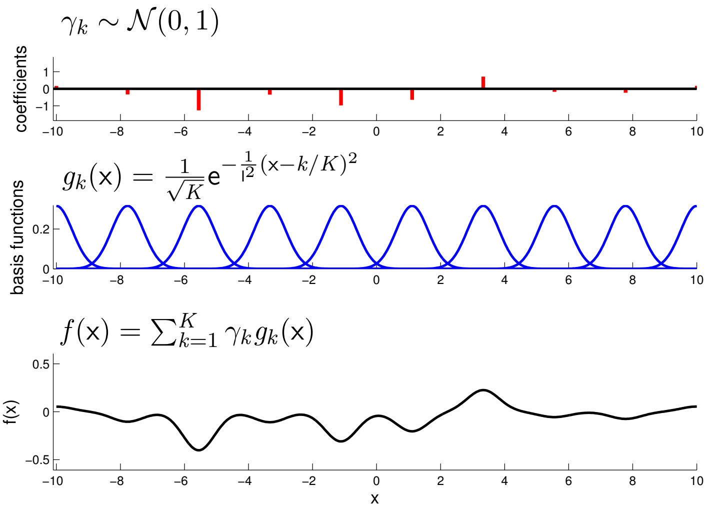

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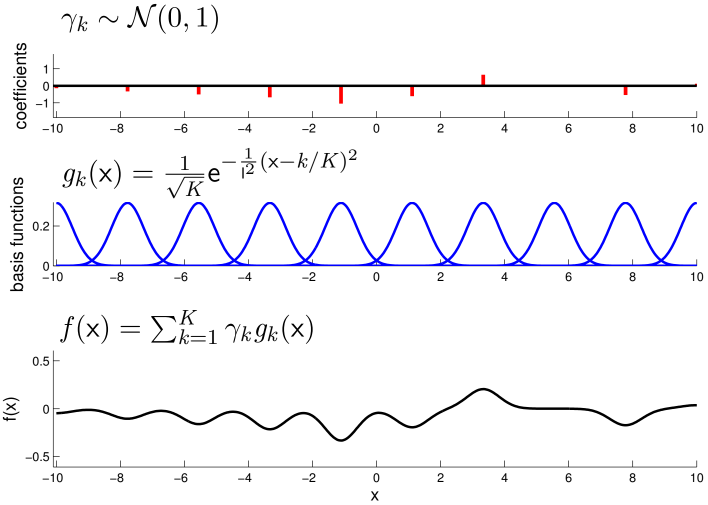

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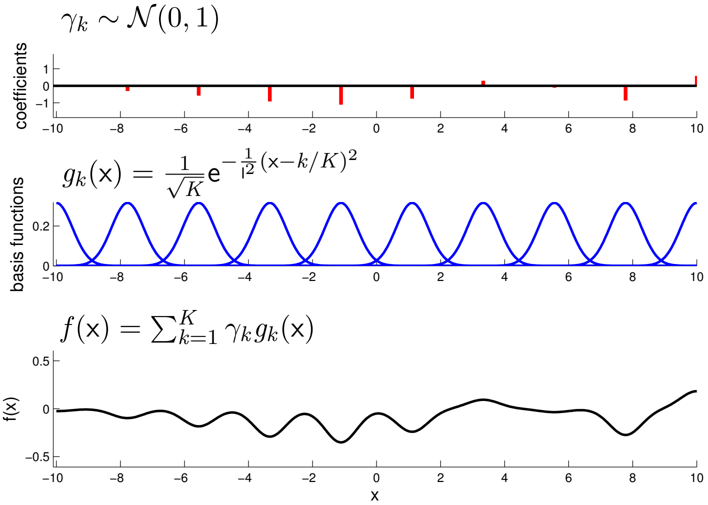

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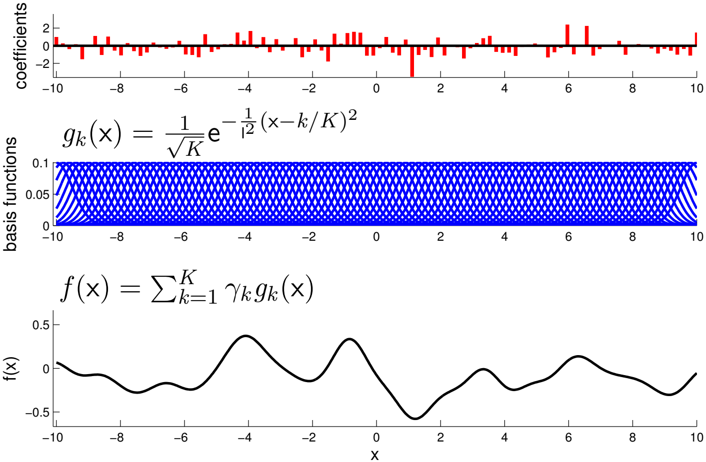

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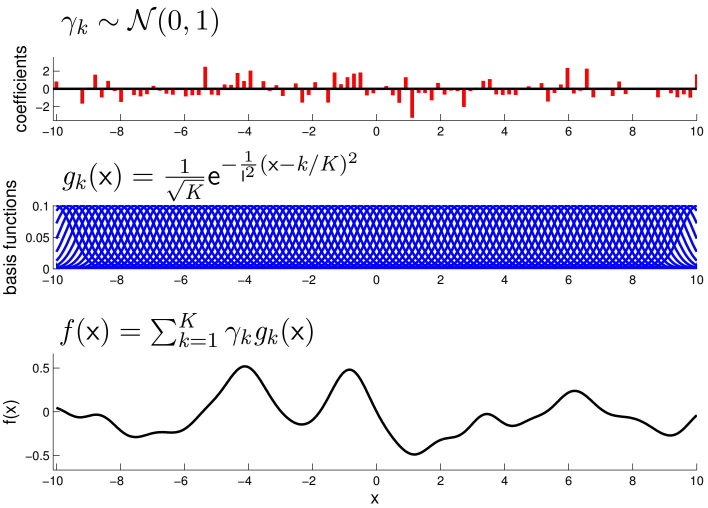

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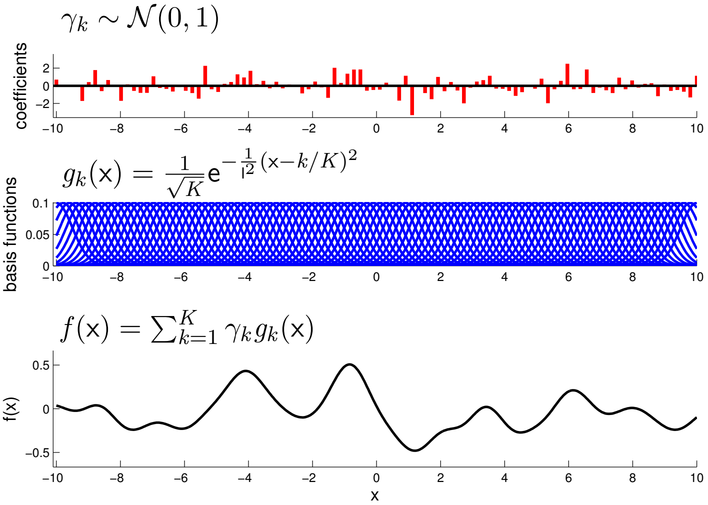

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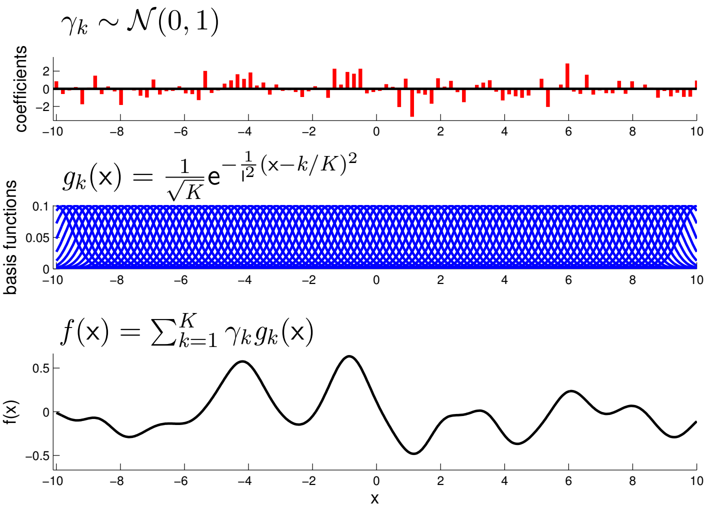

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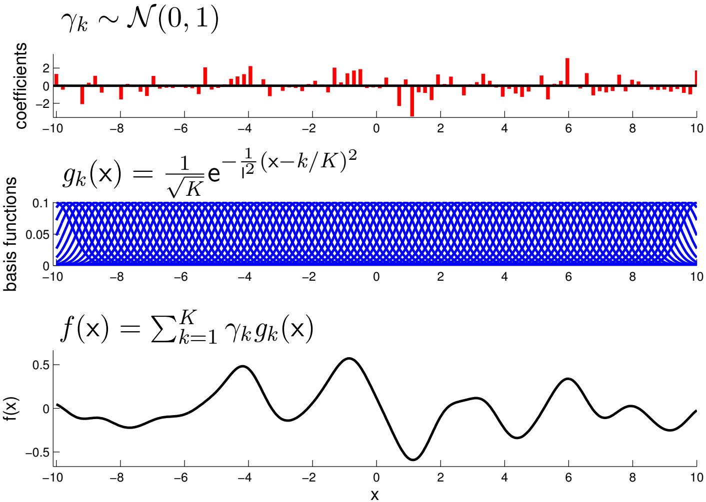

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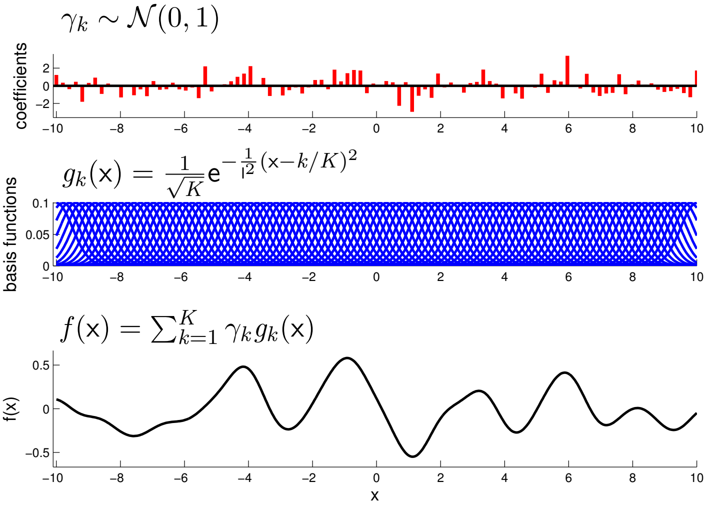

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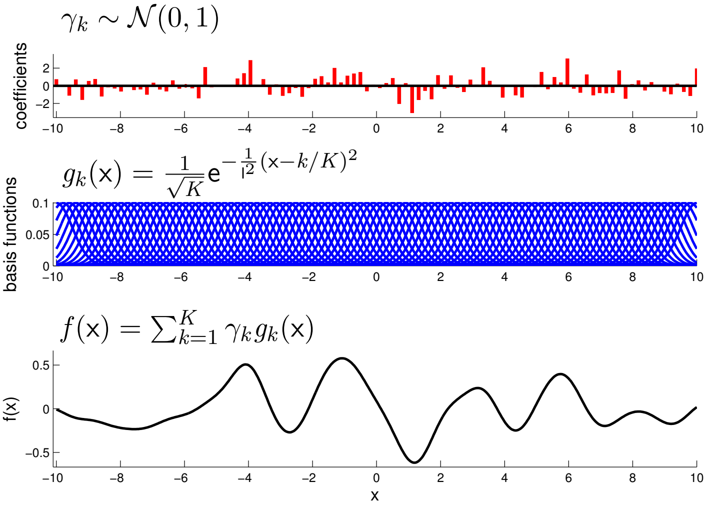

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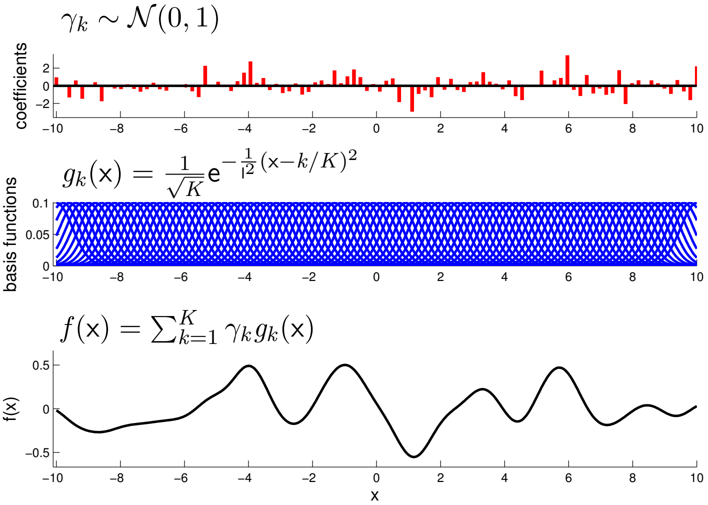

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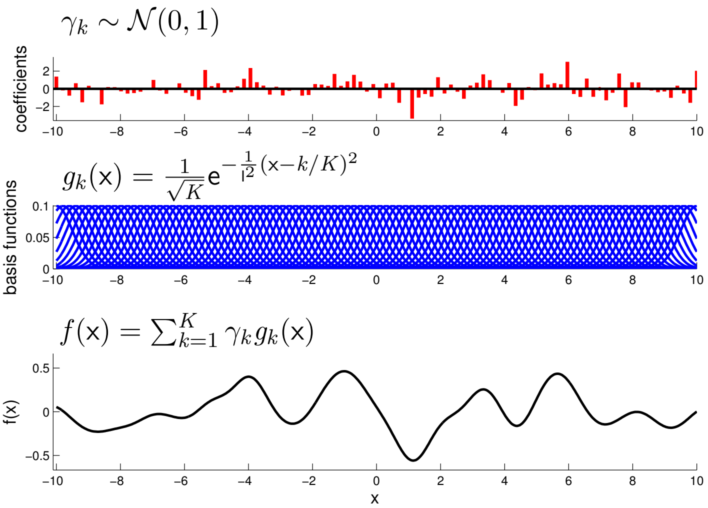

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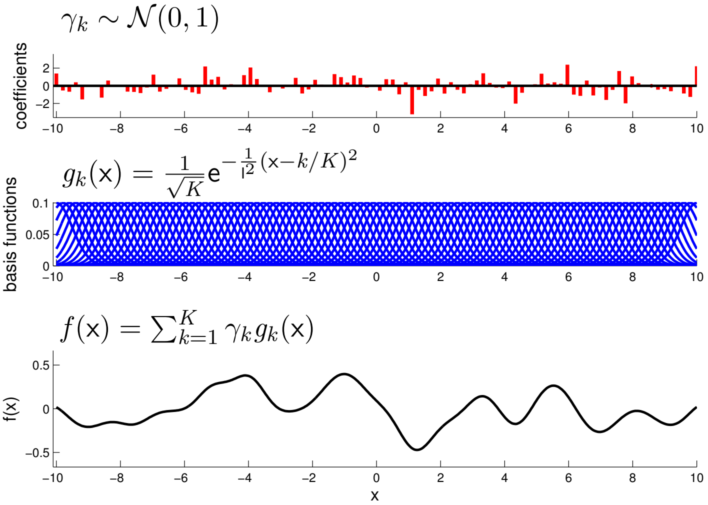

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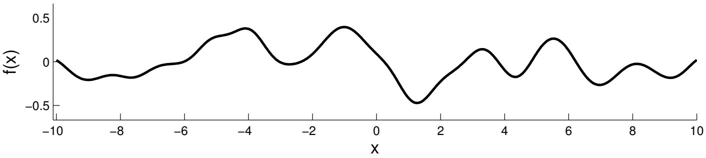

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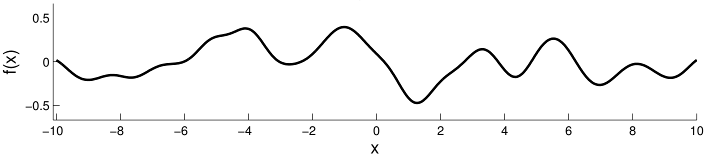

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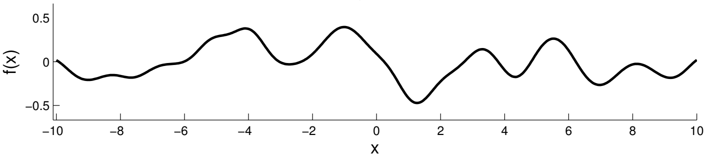

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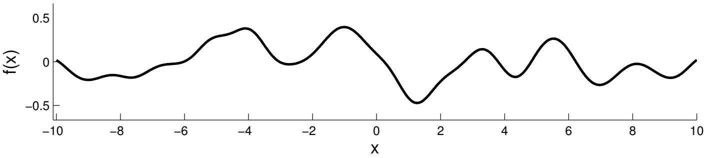

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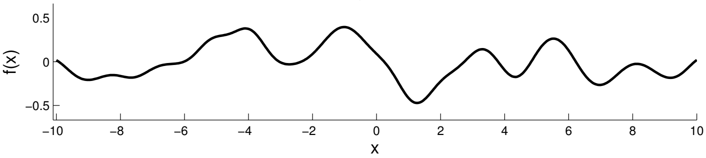

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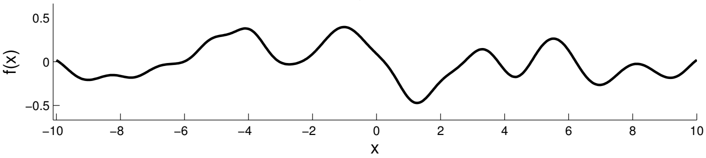

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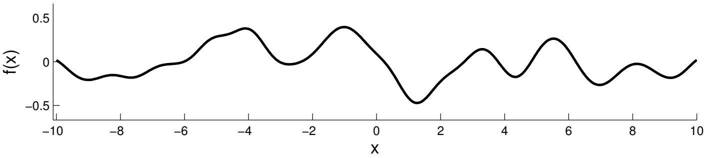

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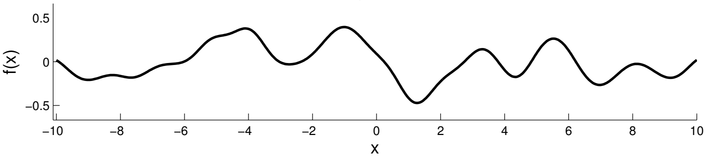

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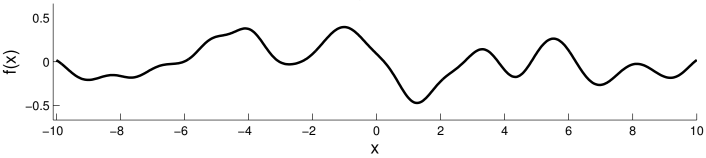

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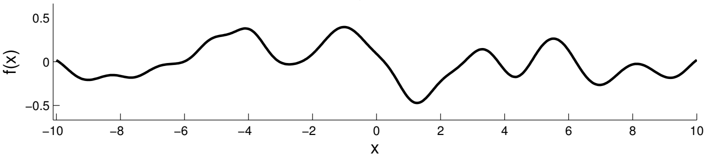

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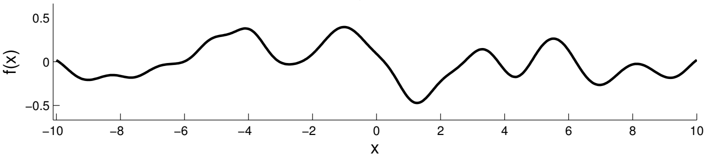
$$\begin{aligned} \mathsf{K}(\mathsf{x},\mathsf{x}') &= \textstyle\sum_k g_k(\mathsf{x}) g_k(\mathsf{x}') \\ &= \frac{1}{K} \textstyle\sum_k \mathsf{e}^{-\frac{1}{\mathsf{l}^2}(\mathsf{x}-k/K)^2 - \frac{1}{\mathsf{l}^2}(\mathsf{x}'-k/K)^2} \\ &\underset{K\to\infty}{\longrightarrow} \int du \;\; \mathsf{e}^{-\frac{1}{\mathsf{l}^2}(\mathsf{x}-u)^2 - \frac{1}{\mathsf{l}^2}(\mathsf{x}'-u)^2} \end{aligned}$$



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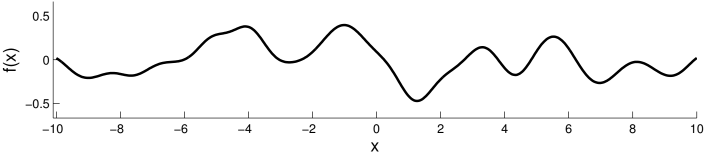
$$\xrightarrow[K \to \infty]{} \int du \;\; \mathsf{e}^{-\frac{1}{\mathsf{l}^2}(\mathsf{x}-u)^2 - \frac{1}{\mathsf{l}^2}(\mathsf{x}'-u)^2}$$

$$\propto \mathsf{e}^{-\frac{1}{2\mathsf{l}^2}(\mathsf{x}-\mathsf{x}')^2}$$



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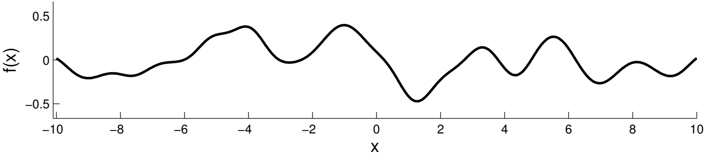

Gaussian processes $\equiv$ models with ∞ parameters

A selection of GP models

probabilistic model	linear mappings	neural network mappings	Gaussian Process mappings
	$f(x) = Wx$	$f(x) = \mathrm{NN}(x; W)$	$f(x) \sim \mathcal{GP}$

A selection of GP models

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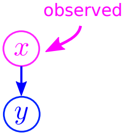
roots

$x \sim \mathcal{N}(\mathbf{0}, \mathrm{I})$

other nodes

$y \,|\, x \sim \mathcal{N}(f(x), \sigma_y^2 \mathrm{I})$

all edges imply a function



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	linear regression		

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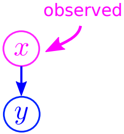

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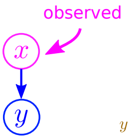

linear regression

(logistic regression)

$y|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$

A selection of GP models

probabilistic model

roots

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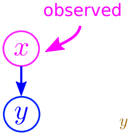

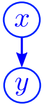

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A selection of GP models

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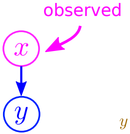

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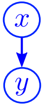

PCA or factor analysis

A selection of GP models

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roots

$$x \sim \mathcal{N}(\mathbf{0}, \mathrm{I})$$

other nodes

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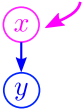
all edges imply a function

observed



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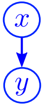

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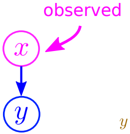
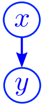
all edges imply a function



linear regression

(logistic regression)

$y|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$



PCA or factor analysis

Gaussian auto-regressive (or Markov) model

A selection of GP models

probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$

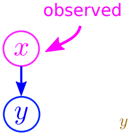
roots

$x \sim \mathcal{N}(\mathbf{0}, \mathrm{I})$

other nodes

$y|x \sim \mathcal{N}(f(x), \sigma_y^2 \mathrm{I})$

all edges imply a function



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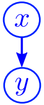

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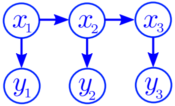

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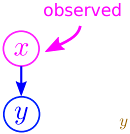

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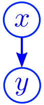

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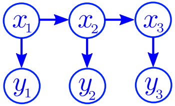


linear Gaussian state space model (LGSSM)

A selection of GP models

probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$

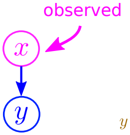
roots

$x \sim \mathcal{N}(\mathbf{0}, \mathrm{I})$

other nodes

$y|x \sim \mathcal{N}(f(x), \sigma_y^2 \mathrm{I})$

all edges imply a function



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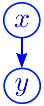
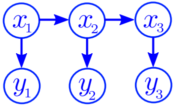


PCA or factor analysis

Gaussian auto-regressive (or Markov) model



linear Gaussian state space model (LGSSM)

A selection of GP models

roots

$x \sim \mathcal{N}(\mathbf{0}, \mathrm{I})$

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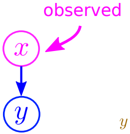
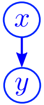
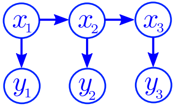
probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$
	linear regression (logistic regression) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	neural network regression (NN classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	
	PCA or factor analysis	variational auto-encoder (VAE) (deep generative model, DGM)	
	Gaussian auto-regressive (or Markov) model	neural auto-regressive density estimation (NADE)	
	linear Gaussian state space model (LGSSM)	recurrent neural latent variable model	

A selection of GP models

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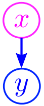
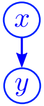
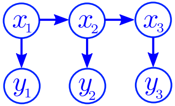
all edges imply a function

probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$
	linear regression (logistic regression) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	neural network regression (NN classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	bad term for a model
	PCA or factor analysis	variational auto-encoder (VAE) (deep generative model, DGM)	
	Gaussian auto-regressive (or Markov) model	neural auto-regressive density estimation (NADE)	
	linear Gaussian state space model (LGSSM)	recurrent neural latent variable model	

A selection of GP models

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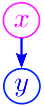
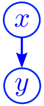
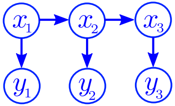
$y \,|\, x \sim \mathcal{N}(f(x), \sigma_y^2 \mathrm{I})$

all edges imply a function

probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$
observed 	linear regression (logistic regression) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	neural network regression (NN classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	
	PCA or factor analysis	variational auto-encoder (VAE) (deep generative model, DGM) bad term for a model	
	Gaussian auto-regressive (or Markov) model	neural auto-regressive density estimation (NADE)	
	linear Gaussian state space model (LGSSM)	recurrent neural latent variable model	

A selection of GP models

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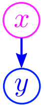
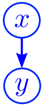
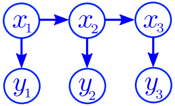
all edges imply a function

probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$
observed 	linear regression (logistic regression) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	neural network regression (NN classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	Gaussian Process regression (GP classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$
	PCA or factor analysis	variational auto-encoder (VAE) (deep generative model, DGM) — bad term for a model	Gaussian Process latent variable model
	Gaussian auto-regressive (or Markov) model	neural auto-regressive density estimation (NADE)	Gaussian process auto-regressive model (GPAR)
	linear Gaussian state space model (LGSSM)	recurrent neural latent variable model	Gaussian process state-space model (GP-SSM)

A selection of GP models

roots

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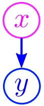
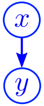
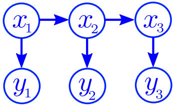
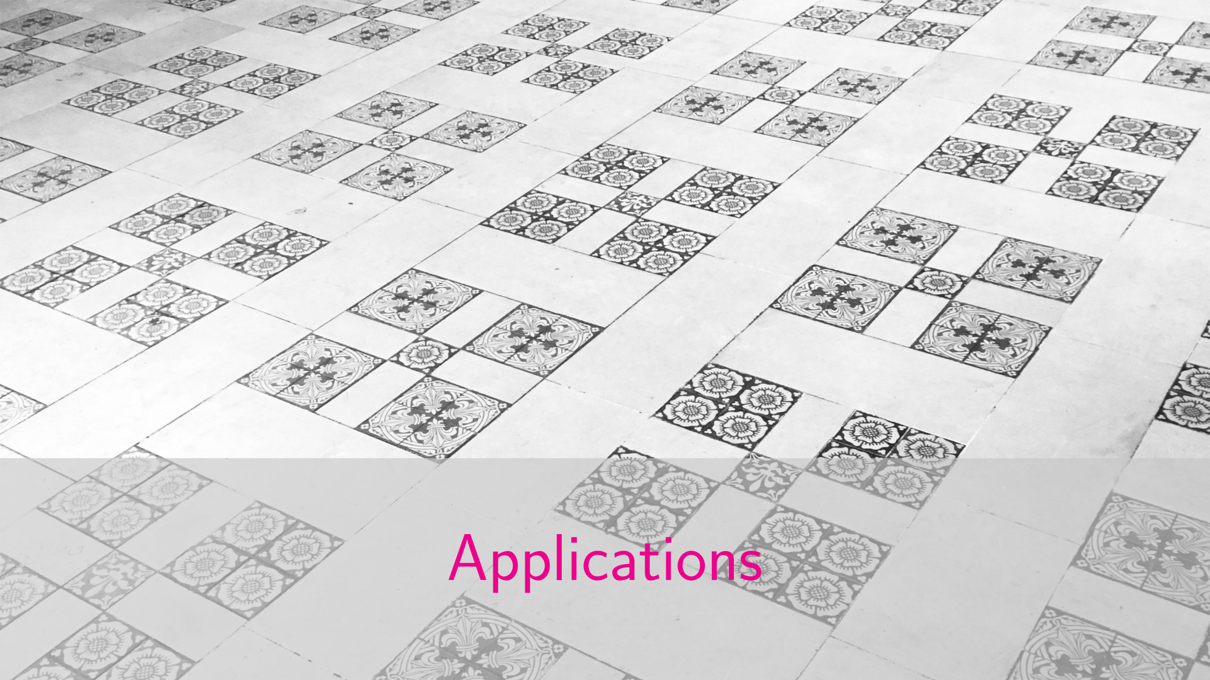
all edges imply a function

probabilistic model	linear mappings $f(x) = Wx$	neural network mappings $f(x) = \mathrm{NN}(x; W)$	Gaussian Process mappings $f(x) \sim \mathcal{GP}$
	linear regression (logistic regression) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	neural network regression (NN classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$	Gaussian Process regression (GP classifcation) $y\|x = \mathrm{Bern}(\mathrm{softmax}[f(x)])$
	PCA or factor analysis	variational auto-encoder (VAE) (deep generative model, DGM) bad term for a model	Gaussian Process latent variable model used inference networks in 2005
	Gaussian auto-regressive (or Markov) model	neural auto-regressive density estimation (NADE)	Gaussian process auto-regressive model (GPAR)
	linear Gaussian state space model (LGSSM)	recurrent neural latent variable model	Gaussian process state-space model (GP-SSM)



Applications

What are Gaussian Processes good for?

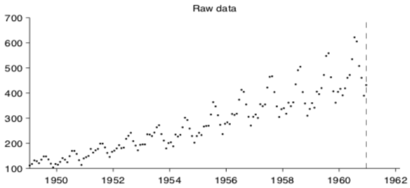
Strengths

- **interpretable** machine learning (covariance functions specify easy-to-explain high-level properties of functions)
- **data-efficient** machine learning (non-parametric + Bayesian $\implies$ lots of flexibility + avoid overfitting)
- **decision making** (well-calibrated uncertainties: knows when it does not know)
- **automated machine learning** including **probabilistic numerics** (regression and classification are rock-solid)

Weaknesses

- **Large numbers of datapoints** ($N \leq 10^5$ unless there is special structure, due to covariance matrix inversion & storage)
- **High-dimensional inputs spaces** ($D \leq 10^2$ unless there is special structure, due to need to compute pair-wise elements of covariance function)

Interpretable auto-ML: the automatic statistician



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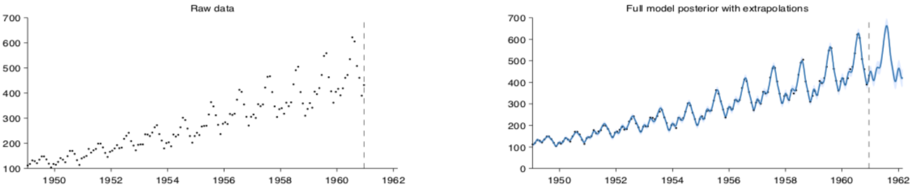

Figure 1: Raw data (left) and model posterior with extrapolation (right)

The structure search algorithm has identified four additive components in the data.

- A linearly increasing function.
- An approximately periodic function with a period of 1.0 years and with approximately linearly increasing amplitude.
- A smooth function.
- Uncorrelated noise with linearly increasing standard deviation.

Interpretable auto-ML: the automatic statistician

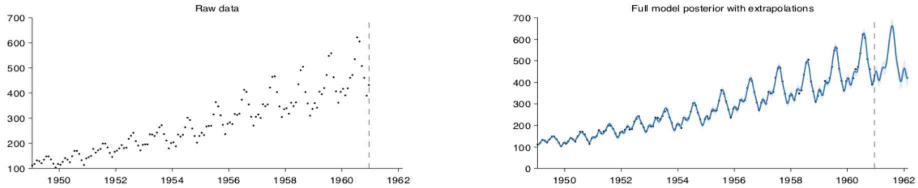

Figure 1: Raw data (left) and model posterior with extrapolation (right)

$$\Sigma(t,t') = \Sigma_1(t,t') + \Sigma_2(t,t') + \Sigma_3(t,t') + \Sigma_4(t,t') + \Sigma_5(t,t')$$

The structure search algorithm has identified four additive components in the data.

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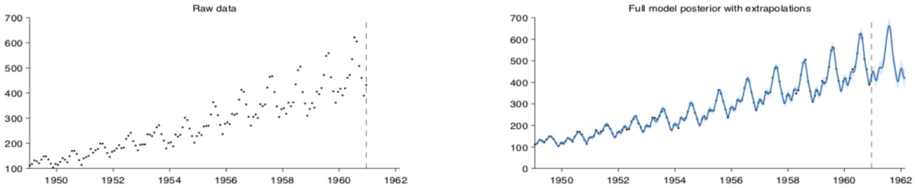

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The structure search algorithm has identified four additive components in the data.

- A linearly increasing function. $\Sigma_1(t,t') = \sigma_m^2 t\, t' + \sigma_c^2$
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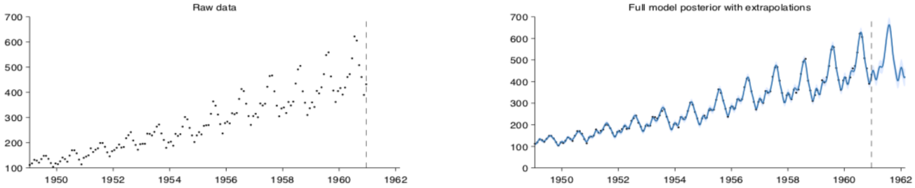
Interpretable auto-ML: the automatic statistician



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The structure search algorithm has identified four additive components in the data.

- A linearly increasing function.

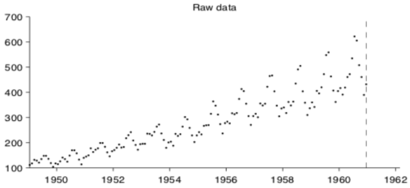
$$\Sigma_1(t,t') = \sigma_m^2 t\, t' + \sigma_c^2$$

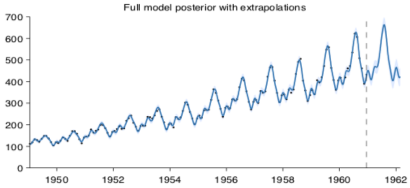
- An approximately periodic function with a period of 1.0 years and with approximately linearly increasing amplitude.

$$\Sigma_2(t,t') = \mathrm{SE}(t,t') \exp(k \cos(\omega(t-t')))$$

- A smooth function.
- Uncorrelated noise with linearly increasing standard deviation.

Interpretable auto-ML: the automatic statistician





$\Sigma_3(t,t') = \mathrm{SE}(t,t')$

Raw data (left) and model posterior with extrapolation (right)

$\Sigma(t,t') = \Sigma_1(t,t') + \Sigma_2(t,t') + \Sigma_3(t,t') + \Sigma_4(t,t') + \Sigma_5(t,t')$

The structure search algorithm has identified four additive components in the data.

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- An approximately periodic function with a period of 1.0 years and with approximately linearly increasing amplitude.
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$\Sigma_1(t,t') = \sigma_m^2 t\, t' + \sigma_c^2$

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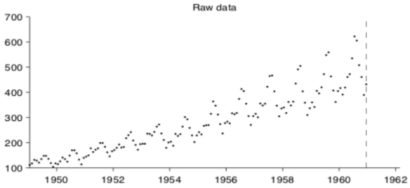
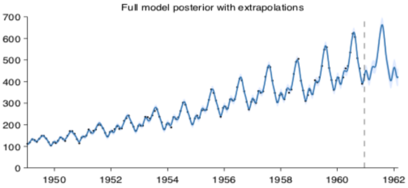
Interpretable auto-ML: the automatic statistician





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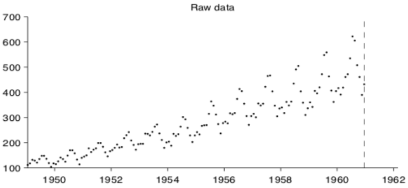
Raw data (left) and model posterior with extrapolation (right)

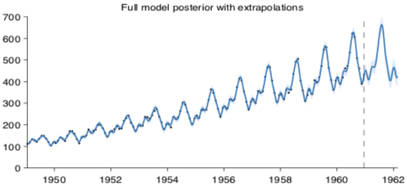
$\Sigma(t, t') = \Sigma_1(t, t') + \Sigma_2(t, t') + \Sigma_3(t, t') + \Sigma_4(t, t') + \Sigma_5(t, t')$

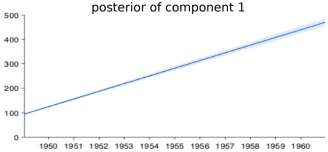
The structure search algorithm has identified four additive components in the data.

- A linearly increasing function. ← $\Sigma_1(t, t') = \sigma_m^2 t\, t' + \sigma_c^2$
- An approximately periodic function with a period of 1.0 years and with approximately linearly increasing amplitude. ← $\Sigma_2(t, t') = \text{SE}(t, t') \exp(k \cos(\omega(t - t')))$
- A smooth function. ← $\Sigma_3(t, t')$
- Uncorrelated noise with linearly increasing standard deviation. ← $\Sigma_4(t, t') = \sigma_y^2 t \delta(t - t')$

Interpretable auto-ML: the automatic statistician



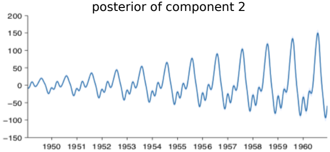


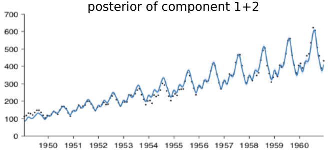


$$\Sigma_1(t,t') = \sigma_m^2 t\, t' + \sigma_c^2$$

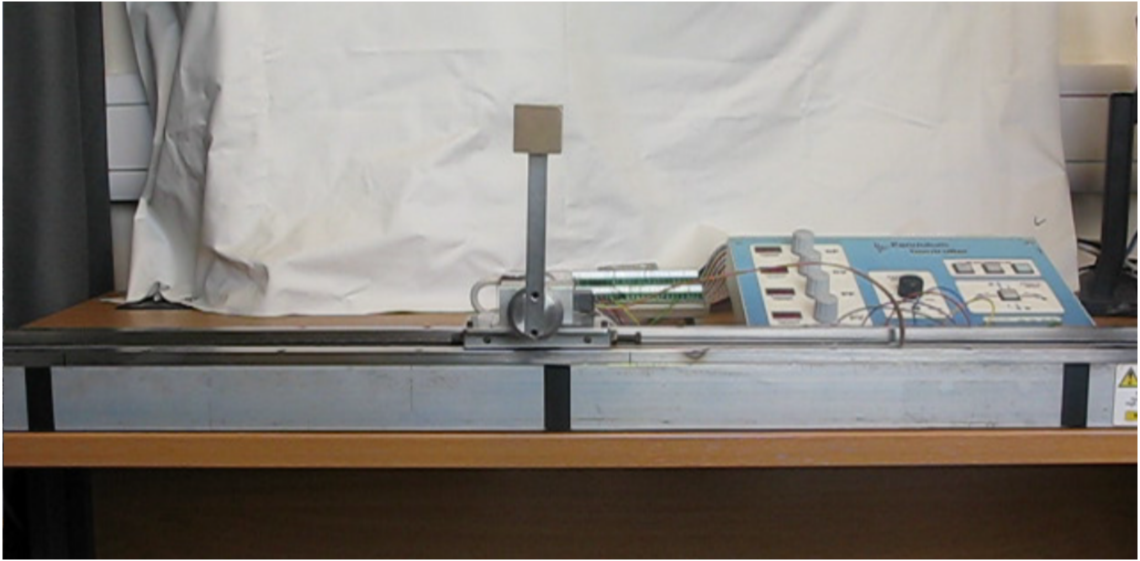
$$\Sigma_2(t,t') = \mathrm{SE}(t,t') \exp(k \cos(\omega(t-t')))$$

$$\Sigma(t,t') = \Sigma_1(t,t') + \Sigma_2(t,t')$$





Data-efficient reinforcement learning: PILCO



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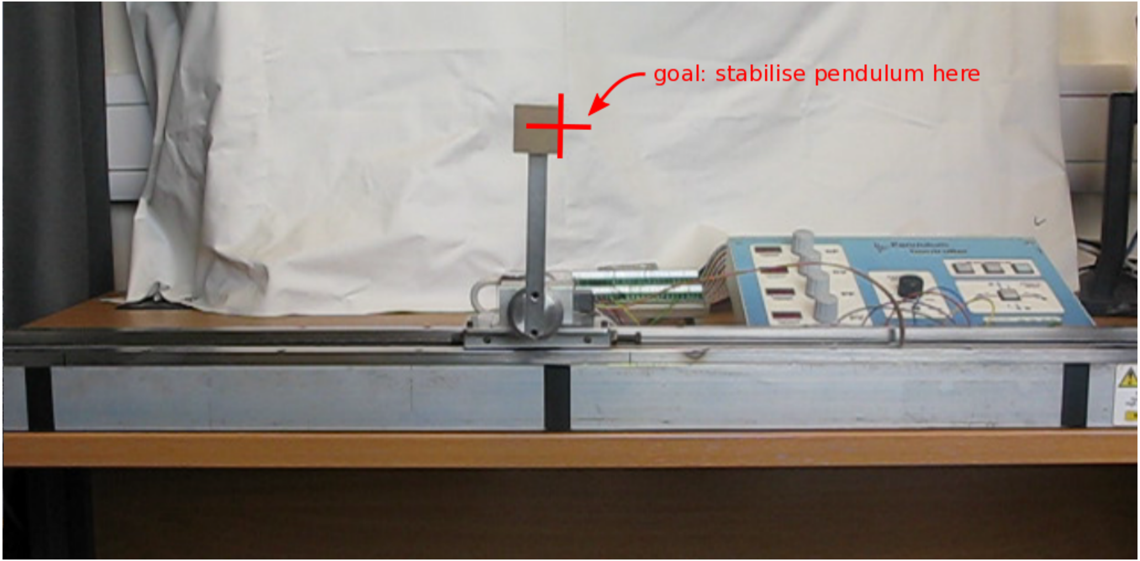

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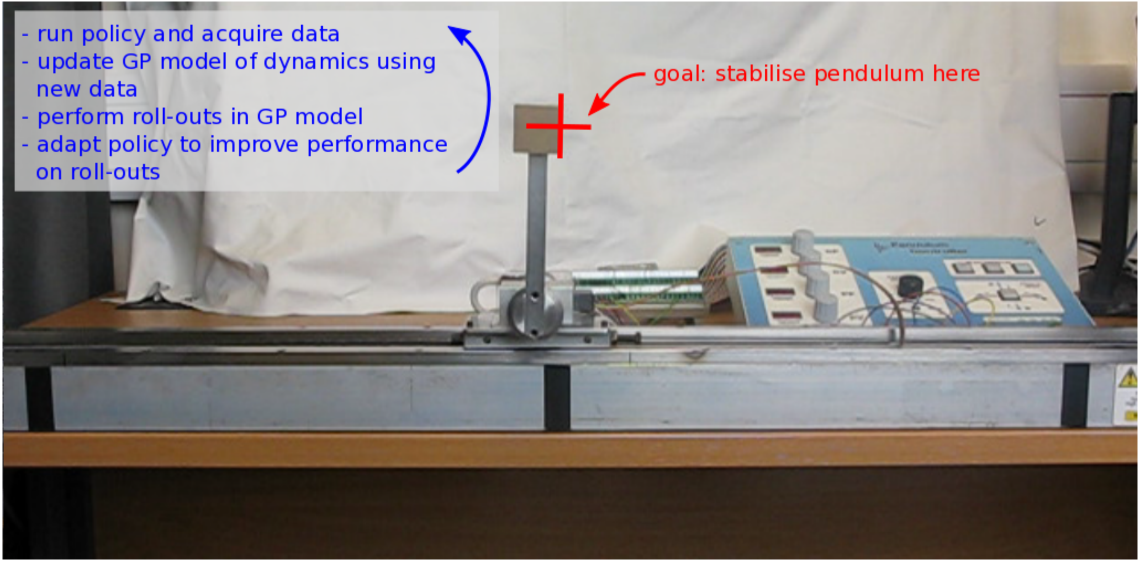
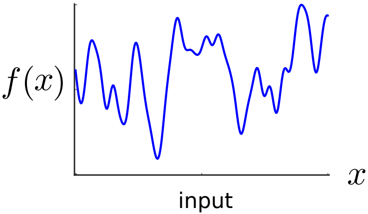


Deep Gaussian Processes

$$y(x) = f(x) + \sigma_{\mathrm{y}}\epsilon$$

$$f(x) = \mathcal{GP}(0, K_f(x, x'))$$



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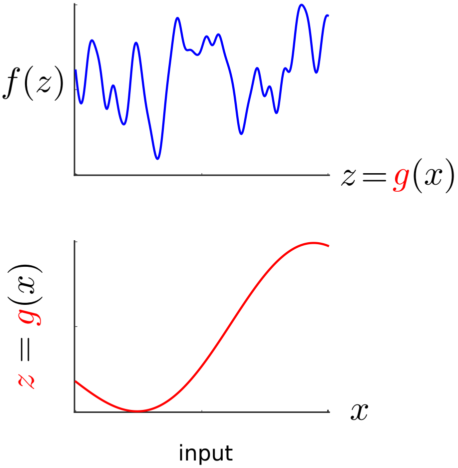

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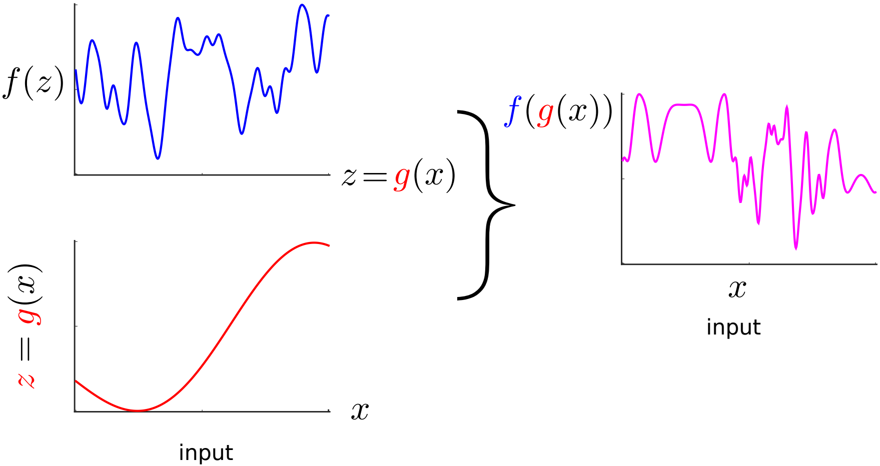

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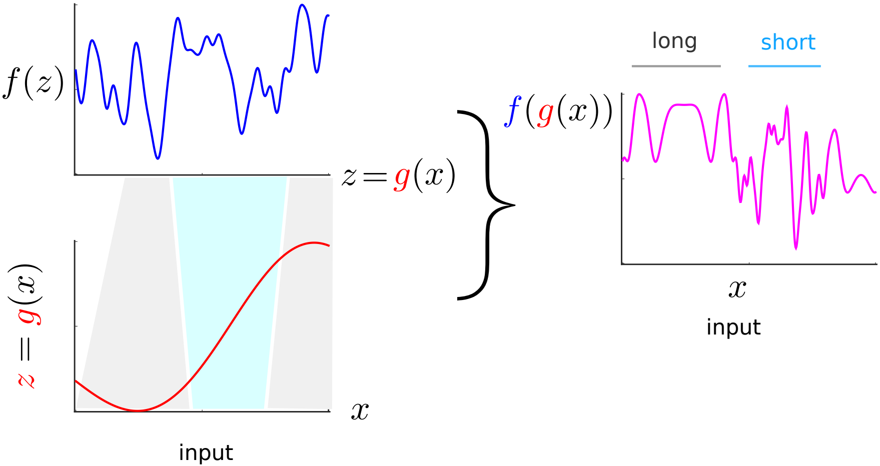

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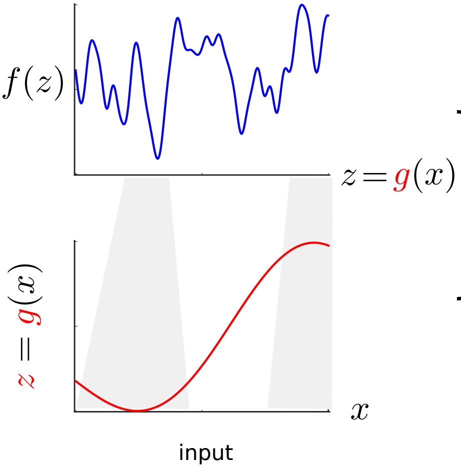
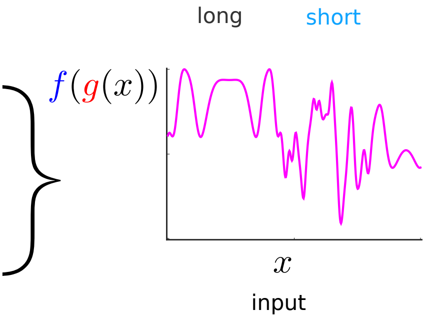
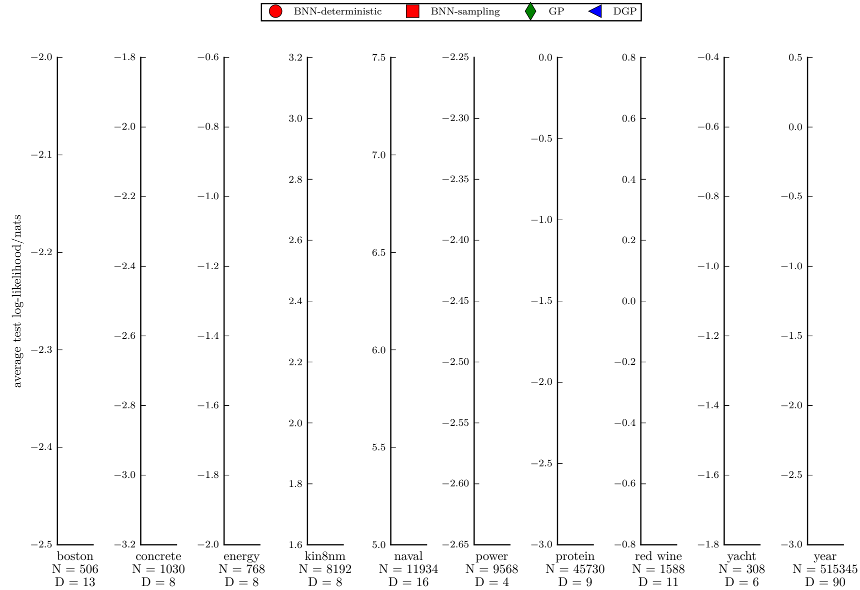




Deep GP perform
automatic kernel design

Experiment: Comparison to Bayesian neural networks [Best results]



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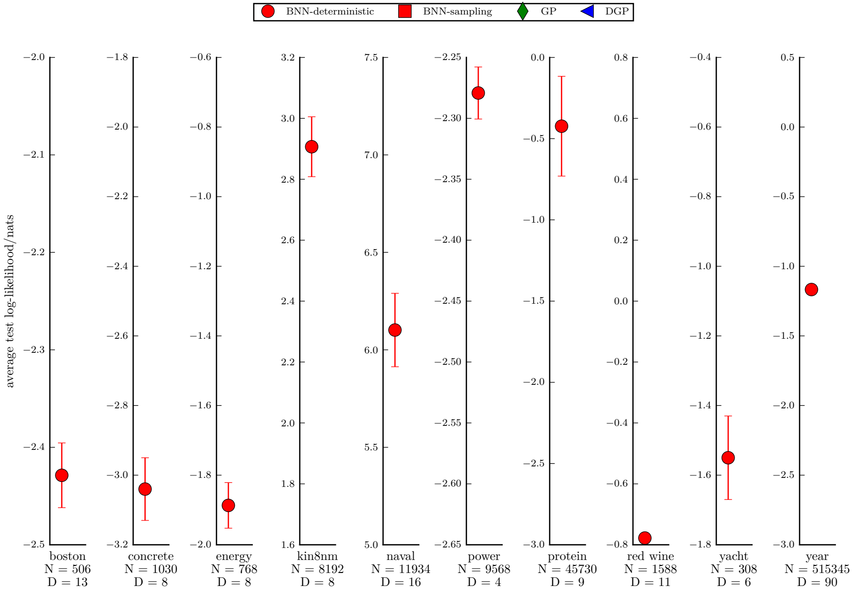

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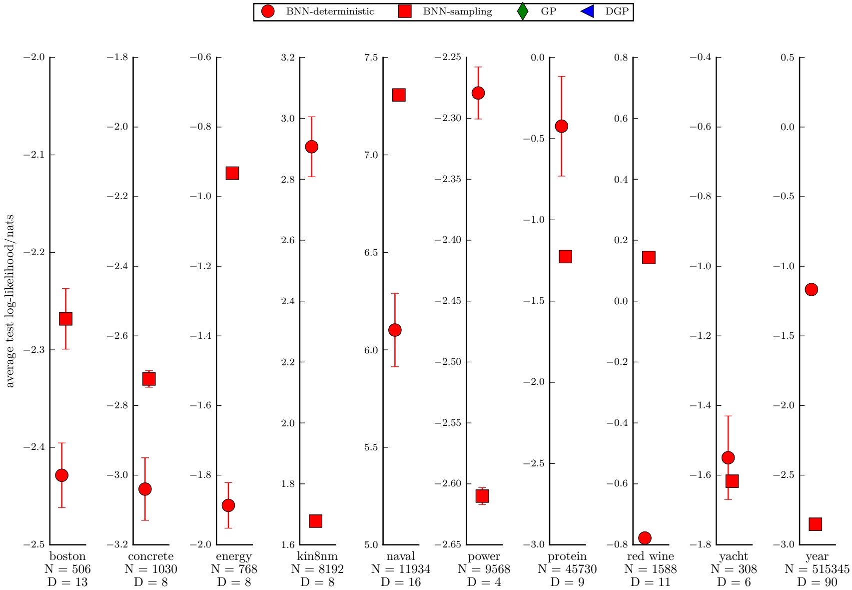

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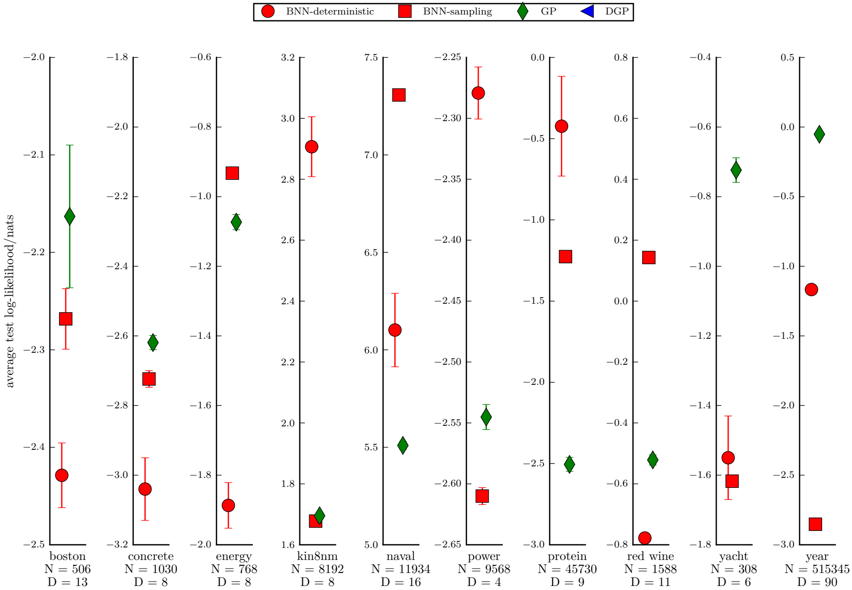

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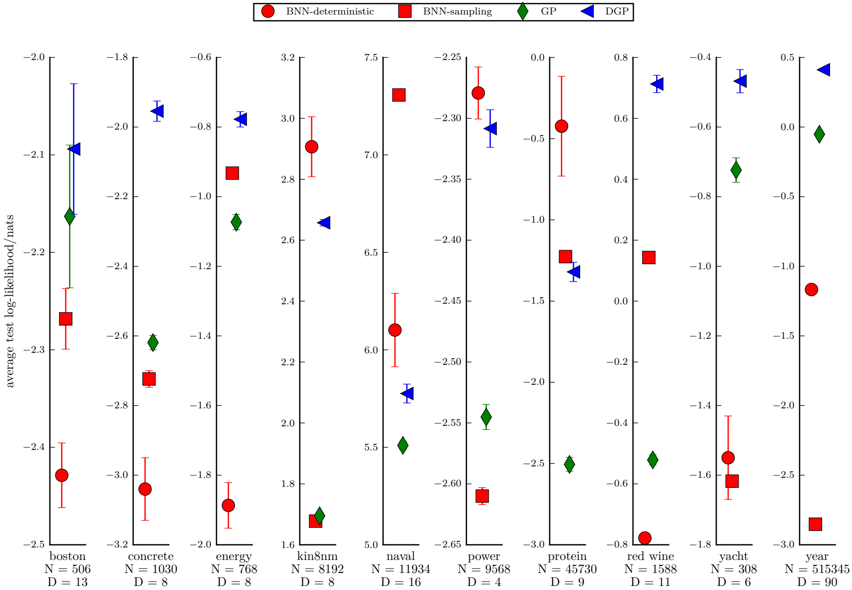
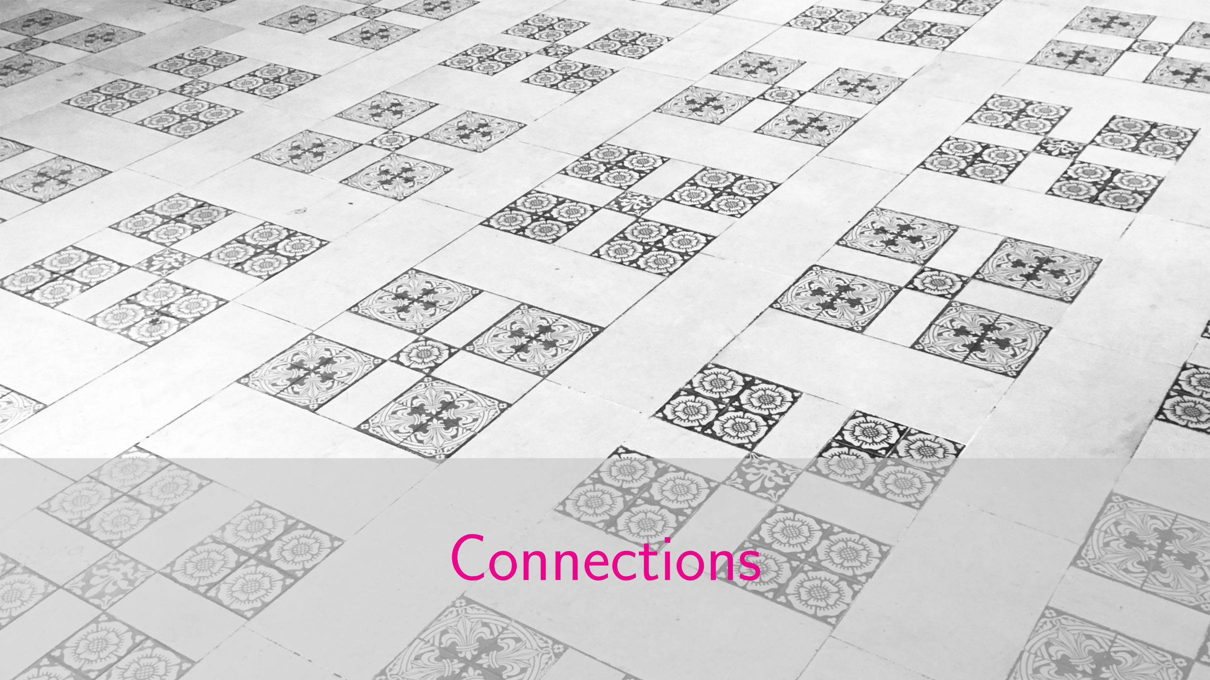
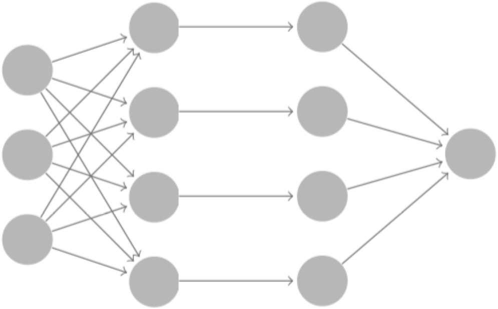




Connections

Infinitely wide neural nets as GPs

inputs	activations	activities	outputs
x	$a = Wx$	$h = \phi(a)$	$f = Vh$



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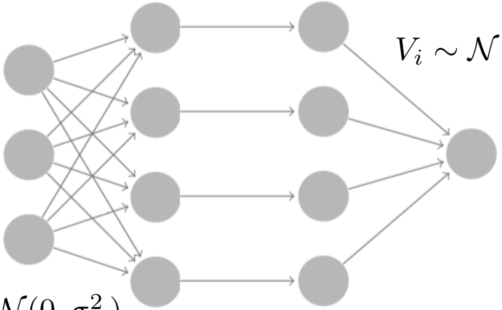

$$V_i \sim \mathcal{N}(0, \sigma_v^2 / D)$$

$$f(x) = \mathrm{NN}(x; W, V)$$

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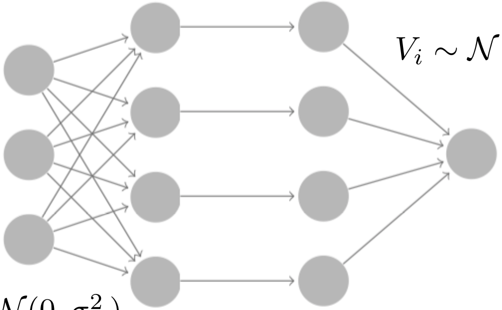

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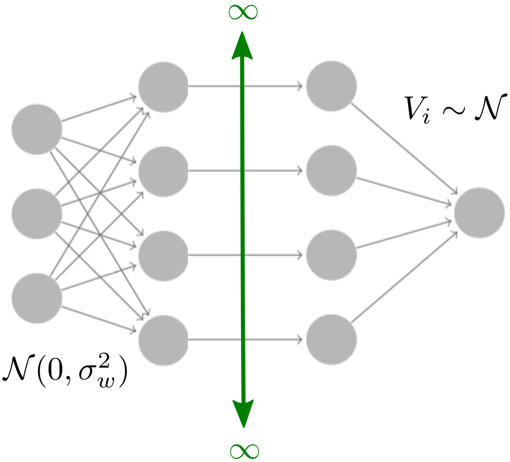

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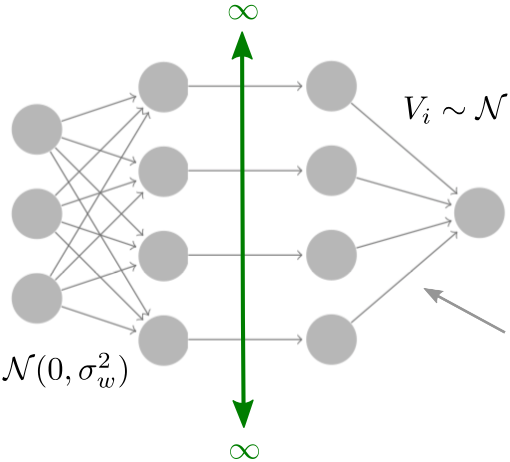

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Neal, 1996

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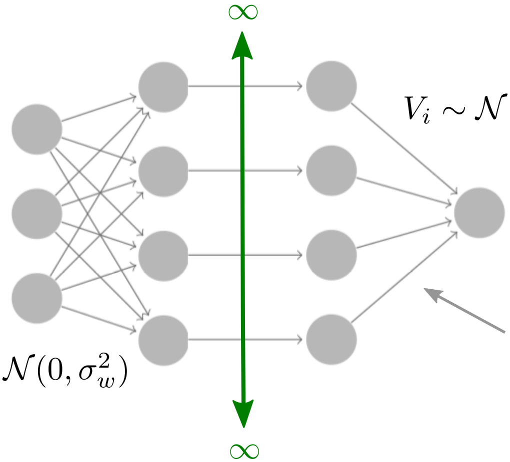

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inputs activations activities activations activities outputs

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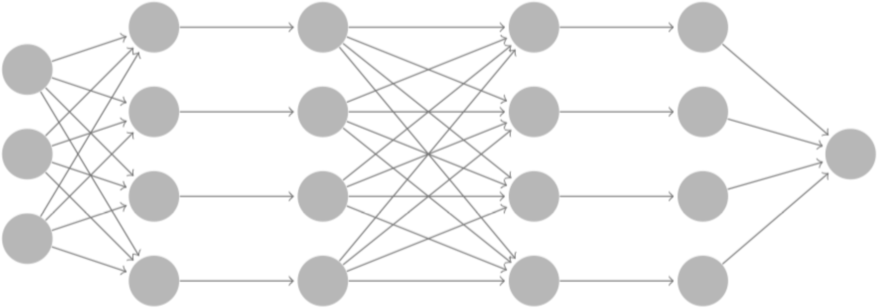

Infinitely wide neural nets as GPs

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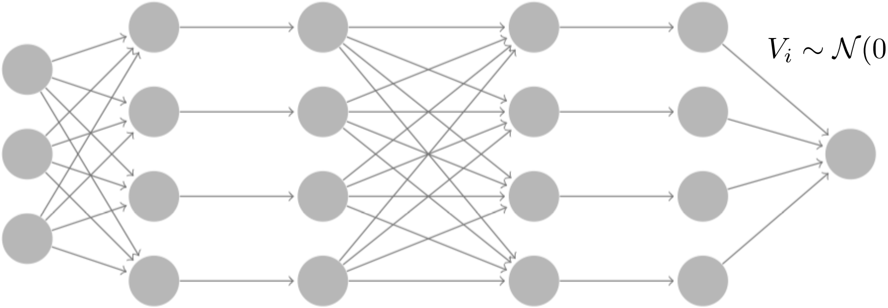
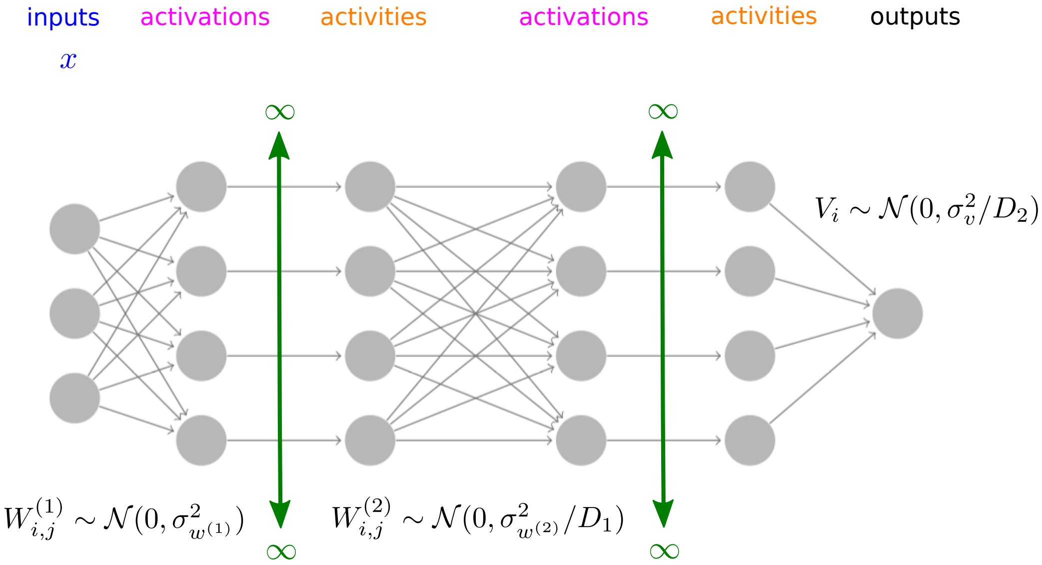


$V_i \sim \mathcal{N}(0, \sigma_v^2 / D_2)$

$W_{i,j}^{(1)} \sim \mathcal{N}(0, \sigma_{w^{(1)}}^2)$

$W_{i,j}^{(2)} \sim \mathcal{N}(0, \sigma_{w^{(2)}}^2 / D_1)$

Infinitely wide neural nets as GPs



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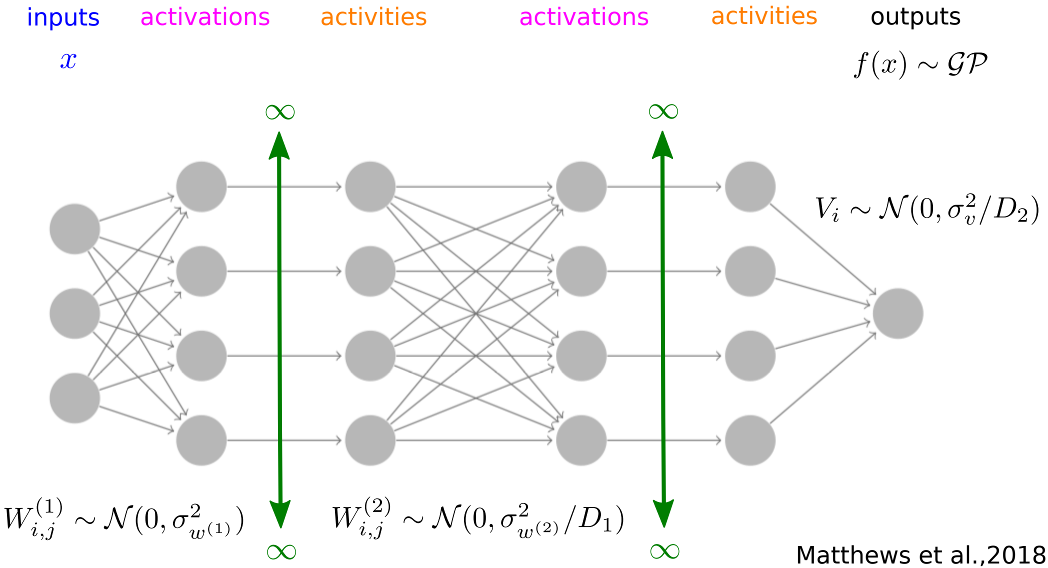

Matthews et al.,2018

Gaussian Processes in Disguise

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- Krigging (geostatistics), splines (curve fitting), moving average processes, time-frequency analysis, ...

References (hyperlinked)

Gaussian Process Models

- Gaussian Process Latent Variable Models for Visualisation of High Dimensional Data
  Lawrence, NIPS, 2005
- Local Distance Preservation in the GP-LVM through Back Constraints, Lawrence and Quinonero-Candela, ICML 2006

The Automatic Statistician

- The Automatic Statistician, Ghahramani et al., (website link)

GPs for Reinforcement Learning and Control

- PILCO: A Model-Based and Data-Efficient Approach to Policy Search, Deisenroth and Rasmussen, ICML 2011

GPs and Neural Networks

- Bayesian Learning for Neural Networks Neal, 1996
- Gaussian Process Behaviour in Wide Deep Neural Networks, Matthews et al., arXiv, 2018