Engineering Mechanics: Machine Learning

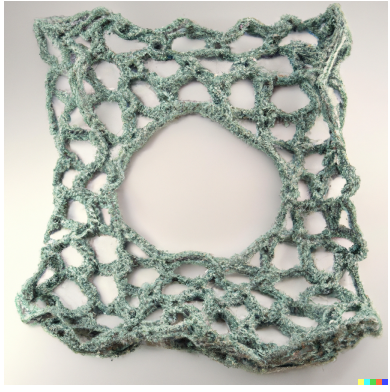
Introduction to ML

Iuri Rocha

A long, long time ago (1.5 years)

Some DALL-E generations we showed at the EM Symposium 2022:

A Finite Element model knitted out of wool



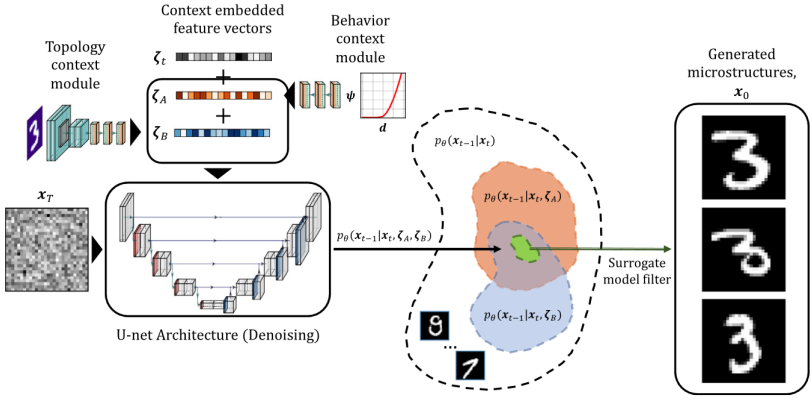
Two teddy bears discovering a new metamaterial

Today

Denoising diffusion for microstructure design:

- Tailored hyperelastic potential

*[Vlassis and Sun (2023), CMAME **413**:116126]*

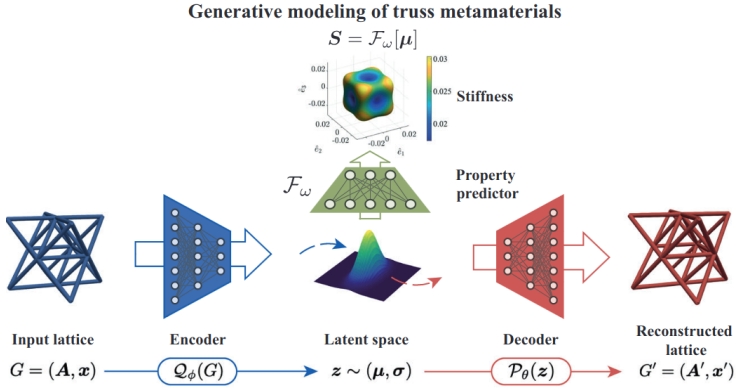


Today

Inverse design of spinodoid metamaterials:

- Tailored stiffness tensor

*[Zheng et al (2023), Nat Comm **2023(14)**:7563]*

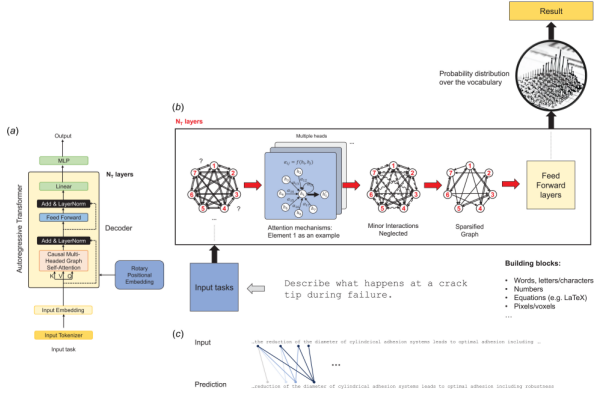


Today

MechGPT, a large language model fine-tuned for mechanics:

- Multimodality, non-trivial connections between different areas of knowledge

*[Buehler (2024), Appl Mech Rev **76(2)**:021001]*

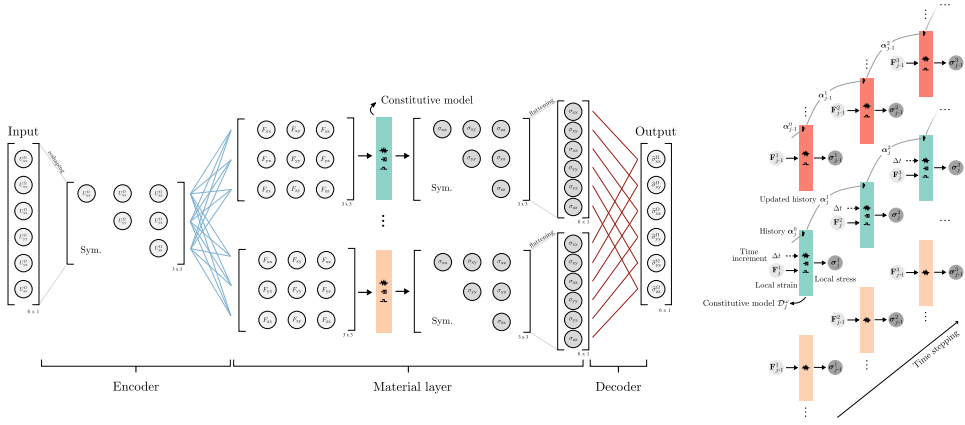


Today

Combining machine learning and physics in creative ways:

- Sparse connectivities, invariances, real material models embedded in architecture

[Maia et al (2024), Coming soon]



Machine Learning — an extremely quick primer

Narrow versus General AI:

- Narrow AI can only perform one specific task ⇐ ML techniques live here
- General AI can perform a multitude of tasks and program itself ⇐ just a dream (for now...)

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Supervised Learning: Tasks with known target outcomes, requires labeled data:

- Regression: Map input features to noisy observations of continuous outputs ⇐ this course
- Classification: Map input features to discrete class labels

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- Dimensionality reduction: Explain the data with a manifold described by continuous latents
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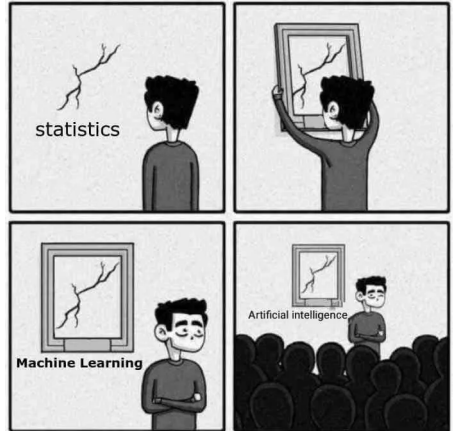
Reinforcement Learning: Learn a task through reward/punishment mechanisms:

- Agent(s) interacting with an environment, evolving interaction policy

Introduction to ML

Contents for this part of the course:

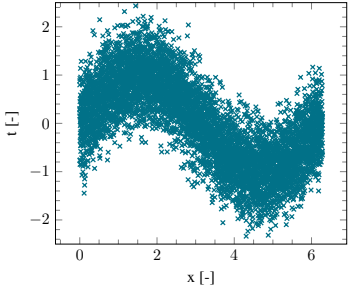
- Decision theory for regression
- Intuitive model building with k-Nearest Neighbors
- Robust model selection, bias-variance tradeoff
- From linear models to neural networks
- Bayesian ML with Gaussian Processes
- The curse of dimensionality, inductive biases



Regression problems

The problem we would like to solve:

- Given: Some complex process $p(\mathbf{x}, t)$, usually highly nonlinear



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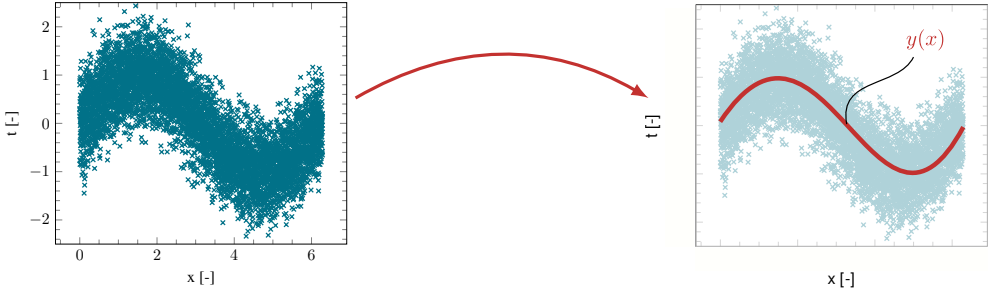

Regression problems

The problem we would like to solve:

- Given: Some complex process $p(\mathbf{x}, t)$, usually highly nonlinear
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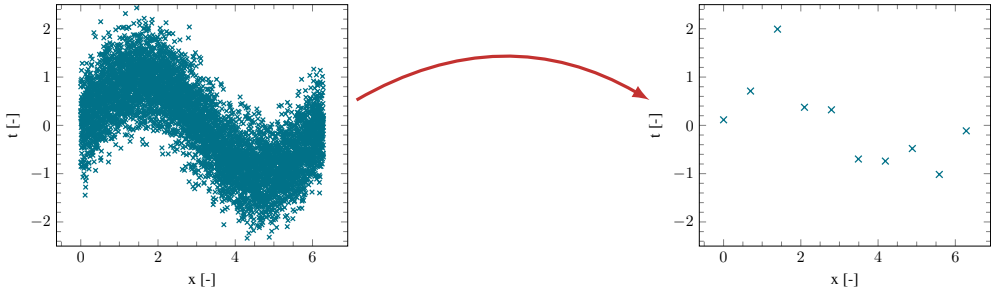
- In practice: We do not know $p(\mathbf{x}, t)$, but only have N observations of it:



Choosing the model $y(x)$

Two main types:

- Parametric models: Knowledge of data encapsulated by a set of parameters: $y(\mathbf{x}, \mathbf{w})$
- Non-parametric models: The whole dataset is directly used to make predictions: $y(\mathbf{x}, \mathcal{D})$

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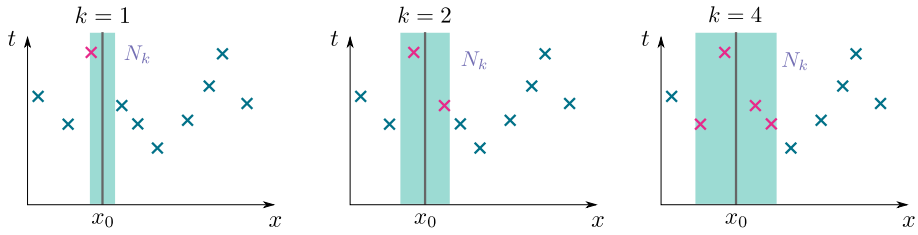
- For a given $\mathbf{x}_0$, we look at a neighborhood N_k around it until we find k data points



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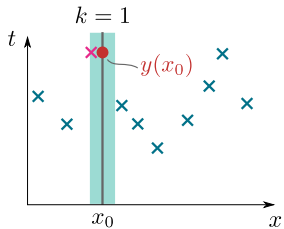
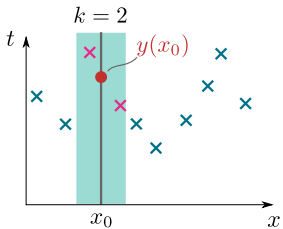
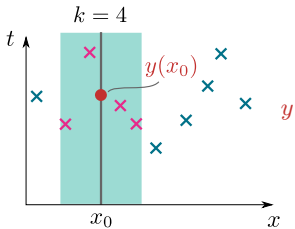
Let us start with a very simple non-parametric model for $y(\mathbf{x})$:

- For a given $\mathbf{x}_0$, we look at a neighborhood N_k around it until we find k data points
- We then average these points, resulting in a k-Nearest Neighbors (kNN) estimator





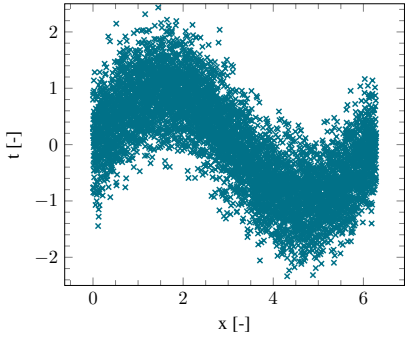


$$y(x_0) = \frac{1}{k} \sum_{x_i \in N_k} t_i$$

Decision Theory for regression

We formalize our problem again from the beginning:

- Given: Some process $p(\mathbf{x}, t)$ we would like to explain with a model
- Goal: Construct a model $y(\mathbf{x})$ that is as close as possible to t



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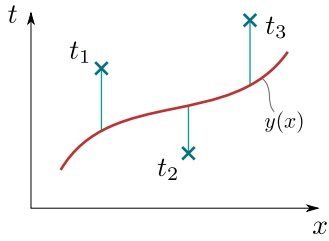
- How to measure this "closeness"? The squared loss function is a popular choice:

$$L(t, y(\mathbf{x})) = (y(\mathbf{x}) - t)^2$$



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$$\mathbb{E}[L] = \int \int (y(\mathbf{x}) - t)^2 \, p(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t$$

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- Solving for the regression function $y(\mathbf{x})$ gives:

$$y(\mathbf{x}) = \int t p(t|x) \, \mathrm{d}t = \mathbb{E}_t[t|\mathbf{x}]$$

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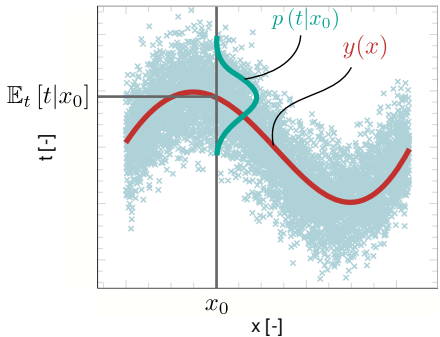

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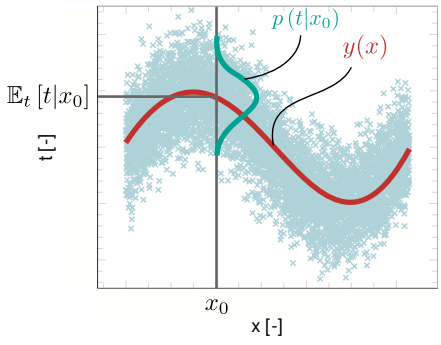
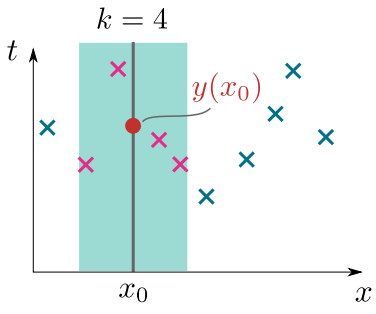


parallel with kNN?

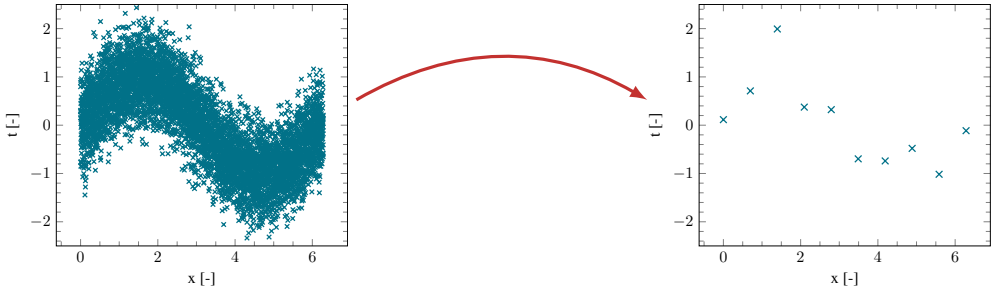


Decision Theory for regression

We formalize our problem again from the beginning:

- Goal: Construct a model $y(\mathbf{x})$ that is as close as possible to t
- In practice we do not know $p\,(x, t)$ exactly and make decisions based on limited data:

$$\int\int (y(\mathbf{x}) - t)^2\, p\,(\mathbf{x}, t)\; \mathrm{d}\mathbf{x}\, \mathrm{d}t \approx \frac{1}{N} \sum_{i}^{N} (y(\mathbf{x}_i) - t_i)^2$$

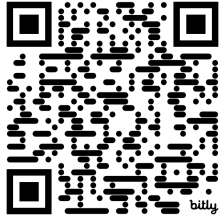


Now let us try this out

Go to bit.ly/engmechml or scan the QR code:

- Look at the first interactive plot
- Change the value of k until you are satisfied with the model
- Change the value of k until the training loss is as small as possible:

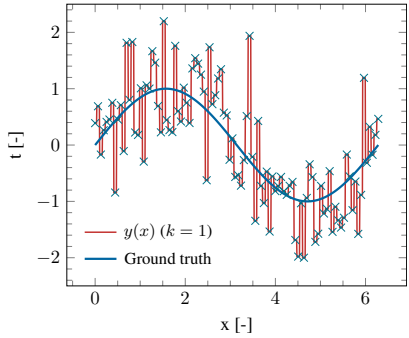
$$\mathbb{E}\left[L\right] \approx \frac{1}{N}\sum_{i}^{N}\left(y(\mathbf{x}_i, k) - t_i\right)^2$$



Overfitting and underfitting

This is the model we get if we are just trying to minimize the training loss:

- Model fits the noise in the dataset and cannot generalize
- The error is exactly zero, but this is not a good model



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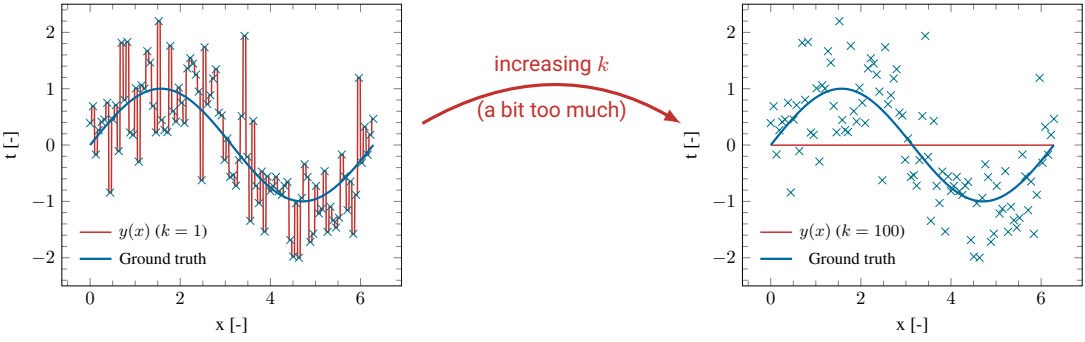
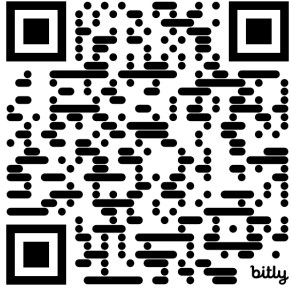
- Too much freedom? What if we increase k?



Let us do this one more time

Go to bit.ly/engmechml or scan the QR code:

- Look at the second interactive plot
- Change the value of k until it is as close as possible to the ground truth



Model selection

In practice we do not know the ground truth, so choosing k is tricky:

- Too low: we fit the noise in the data $\Rightarrow$ overfitting!
- Too high: we oversmooth and lose detail $\Rightarrow$ underfitting!
- The training set cannot be trusted to give us k, it will always lead to $k = 1$

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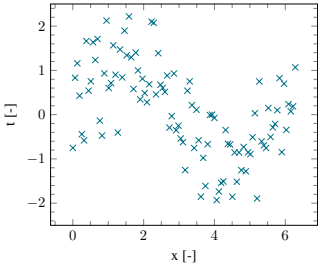
The solution is to introduce a validation dataset:

- A new dataset that cannot be used for training
- We can then use it to find the hyperparameter k:

$$k = \arg\min_{\overline{k}} \frac{1}{N_{\text{val}}} \sum_{i}^{N_{\text{val}}} \left(y(\mathbf{x}_i, \overline{k}) - t_i \right)^2$$

Model selection

But how do we pick a validation set?



100 samples

Model selection

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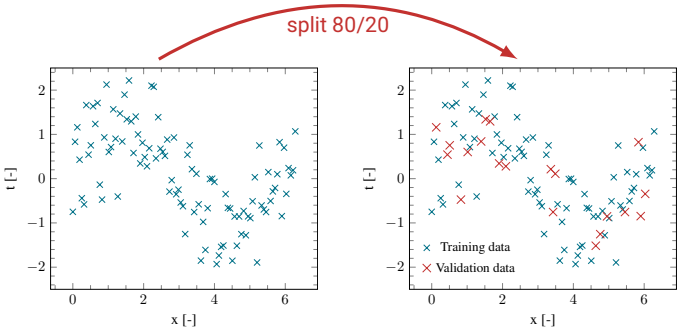

100 samples

80 training samples
20 validation samples

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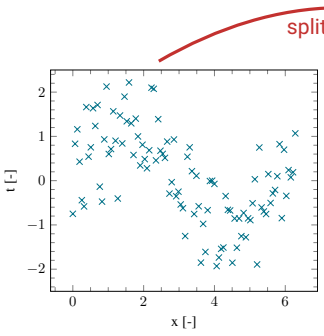

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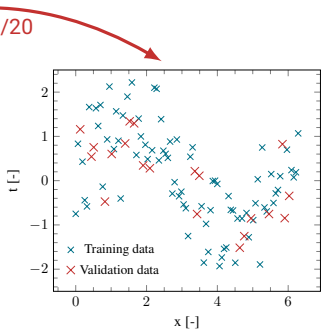
split 80/20



80 training samples
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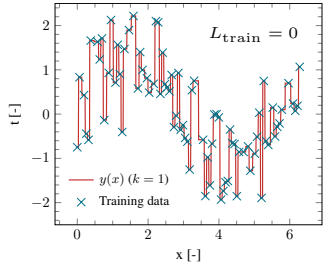
train



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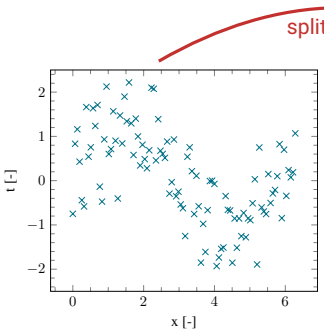

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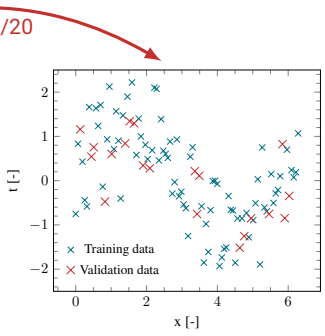

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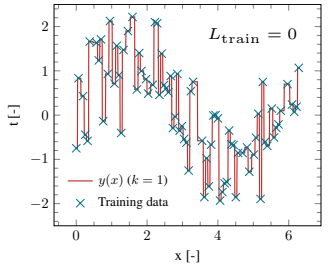
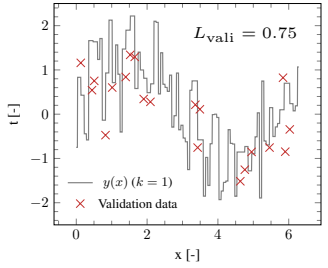
validate

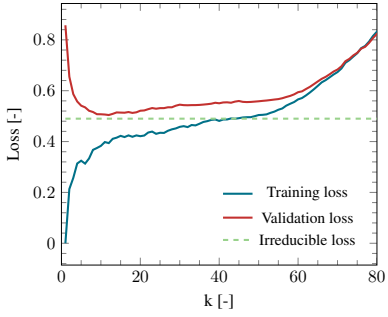




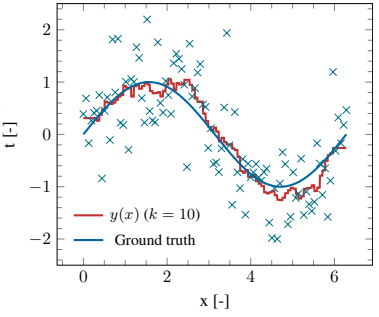
Model selection

The bias-variance tradeoff:

- Overly flexible models have low bias and high variance
- Overly rigid models have high bias and low variance
- We may accept some bias in exchange for a lower variance... but not too much



pick k at minimum loss



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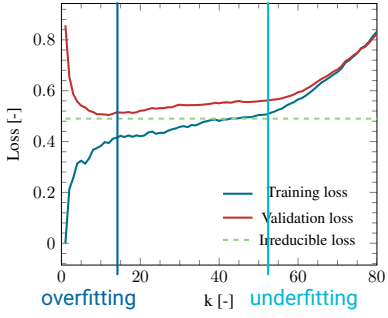

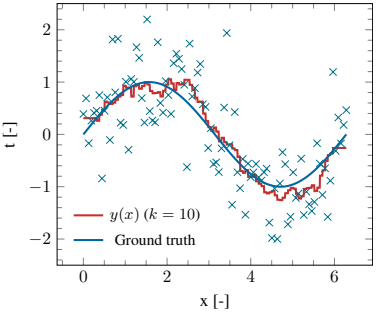

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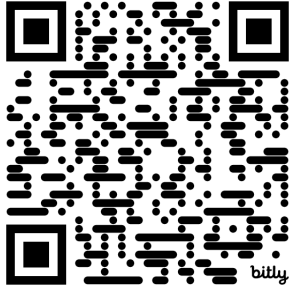
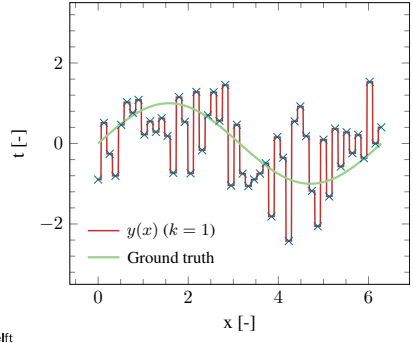


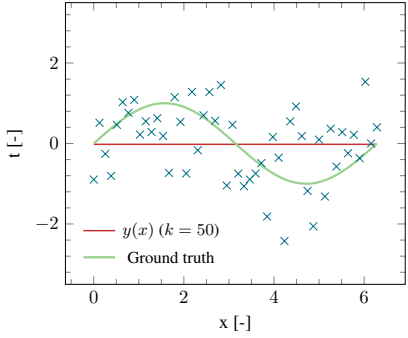
The bias-variance tradeoff

Why do we say flexible models have high variance? A closer look:

- Same example as before, but now 1000 different datasets of $N = 50$ each
- How much does the choice of dataset affect the final model?

$$L(\mathbf{x}) = \underbrace{\left(\mathbb{E}_{\mathcal{D}}\left[y(\mathbf{x}, \mathcal{D})\right] - h(\mathbf{x})\right)^2}_{\text{bias}^2} + \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(y(\mathbf{x}, \mathcal{D}) - \mathbb{E}_{\mathcal{D}}\left[y(\mathbf{x}, \mathcal{D})\right]\right)^2\right]}_{\text{variance}} + \underbrace{\int \left(h\left(\mathbf{x}\right) - t\right)^2 p(t|\mathbf{x})\, \mathrm{d}t}_{\text{irreducible noise}}$$





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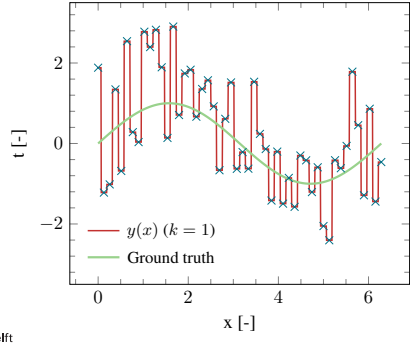

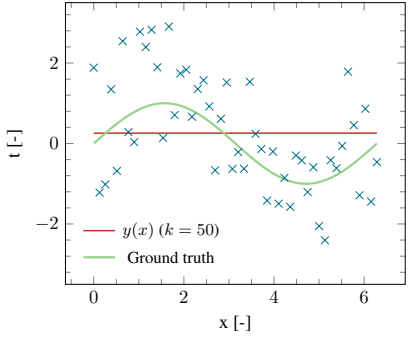

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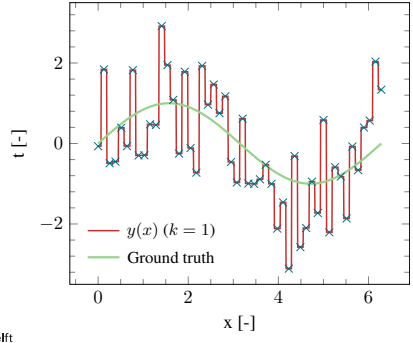

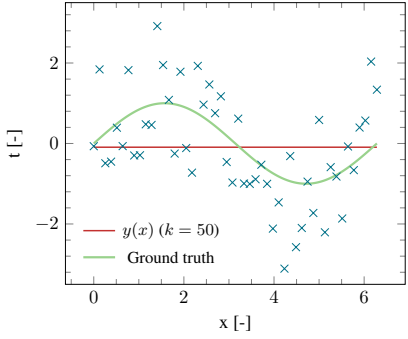

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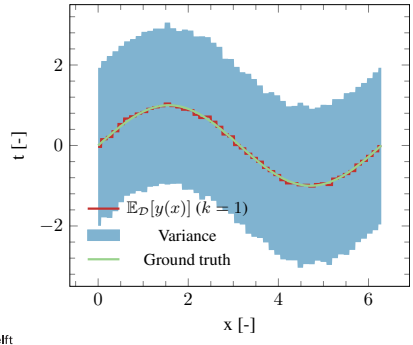

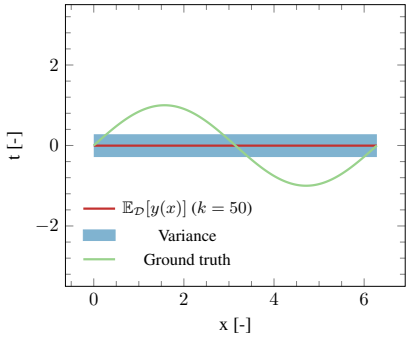

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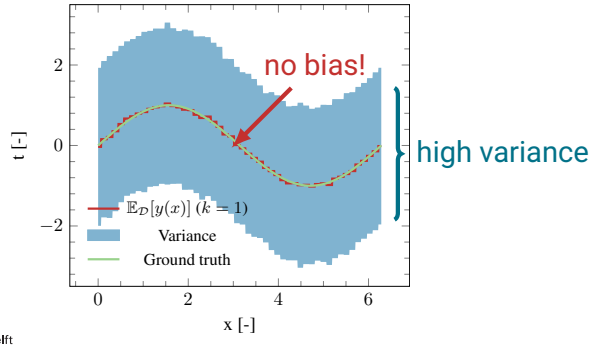

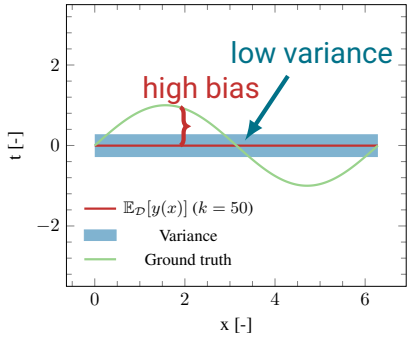

Linear basis function models

Simple linear regression, assuming D input features in $\mathbf{x}$:

- Parametric model, linear in its arguments:

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \cdots + w_D x_D$$

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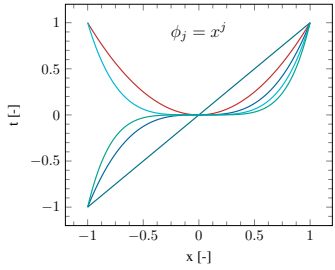
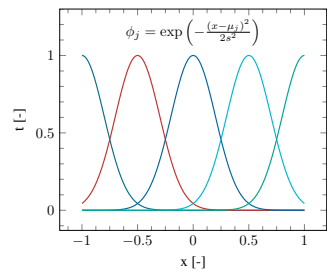


Here we make them more flexible:

- General nonlinear functions of $\mathbf{x}$ as regressors:

$$y(\mathbf{x}, \mathbf{w}) = \sum_j^M w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

- A bias term $\phi_0 = 1$ is usually included in $\boldsymbol{\phi}$
- We are now unshackled from the original dimensionality D



Linear basis function models

Observation model:

- We adopt a parametric model and assume additive Gaussian noise:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon \quad \text{with} \quad \epsilon \sim \mathcal{N}\left(0, \beta^{-1}\right)$$

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We are implicitly assuming:

- Noise is Gaussian
- Response is unimodal

Maximum Likelihood Estimation

Computing the likelihood of our data:

- The probability density of a given value t is:

$$p\left(t \mid \mathbf{w}\right) = \mathcal{N}\left(t \,|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right)$$

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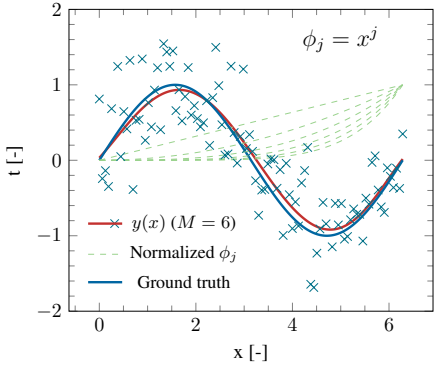
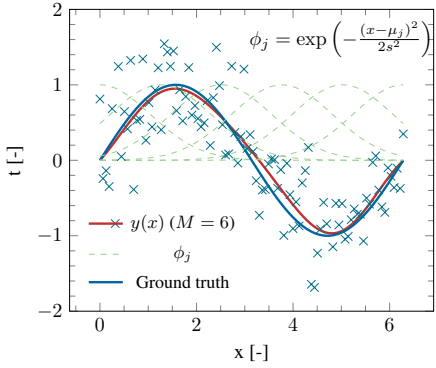
- Maximizing the likelihood is therefore equivalent to minimizing the error in red
- This is where the usual loss function for ML regression comes from

Maximum Likelihood Estimation

How does this look like? An example:

- Dataset with $N = 100$ observations, $M = 6$ basis functions (polynomials or Gaussians)

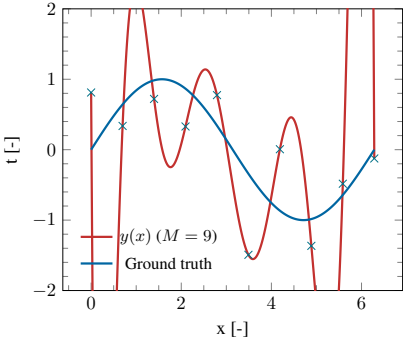


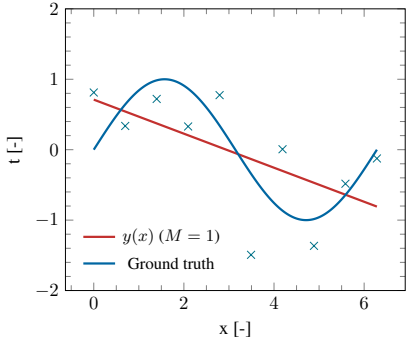


Overfitting and underfitting MLE models

Also here, flexibility is not always a good thing:

- Dataset with $N = 10$ observations, model with complete order M polynomials
- Again a tradeoff between bias and variance





Stochastic Gradient Descent

For now we have trained with the complete dataset at once:

- The error function contains all N data points:

$$E_{\mathcal{D}} = \frac{1}{2} \sum_{n=1}^{N} \left(t_n - \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}_n) \right)^2$$

Situations when it is interesting (or necessary) to deviate from this:

- N is too large and computing $\left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi} \right)^{-1}$ becomes prohibitive
- The model is nonlinear (in $\mathbf{w}$) and $\mathbf{w}_{\mathrm{ML}}$ does not have a closed-form solution
- The dataset is arriving sequentially (e.g. in real time from a sensor)

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Instead of solving directly for $\mathbf{w}_{\mathrm{ML}}$, we can use Gradient Descent:

- Pick a (random) subset $\mathcal{B}$ of the dataset with $N_{\mathcal{B}}$ observations

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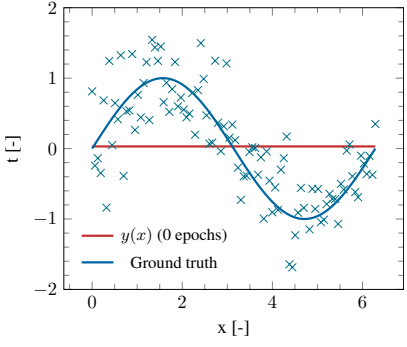
Variations:

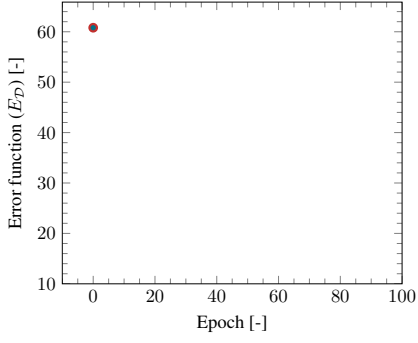
- $N_{\mathcal{B}} = 1$: Online stochastic gradient descent
- $1 < N_{\mathcal{B}} < N$: Minibatch SGD (most popular)
- $N_{\mathcal{B}} = N$: Full batch gradient descent

Stochastic Gradient Descent

An example:

- Same example as before, with $N = 100$ and $M = 6$ polynomial basis functions
- We fix the learning rate $\eta = 0.001$ and minibatch size $N_{\mathcal{B}} = 10$





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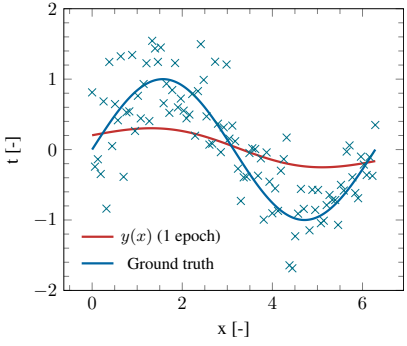

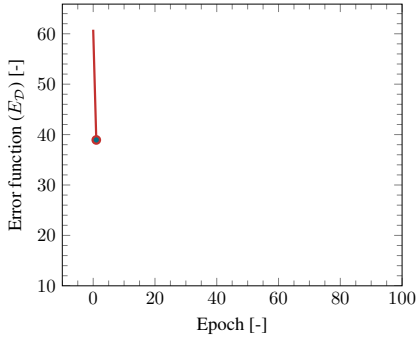

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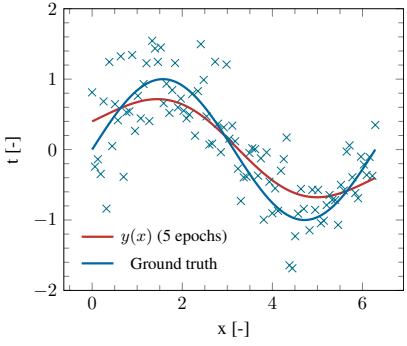

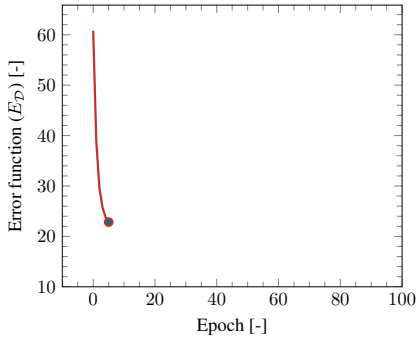

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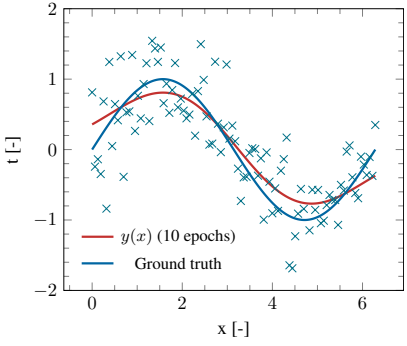

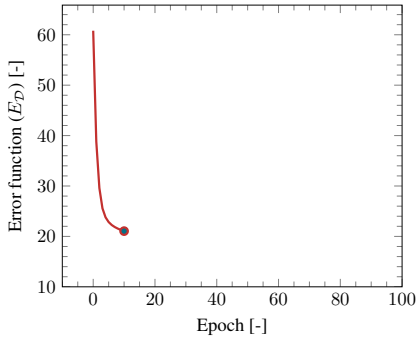

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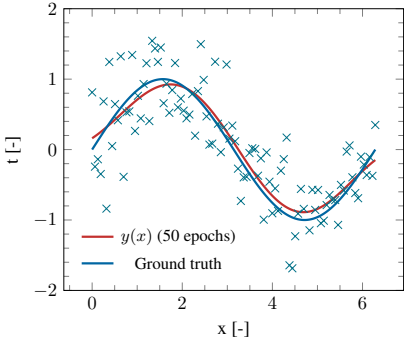

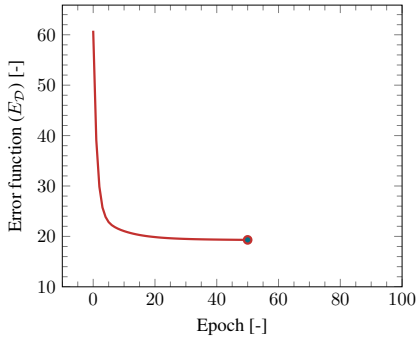

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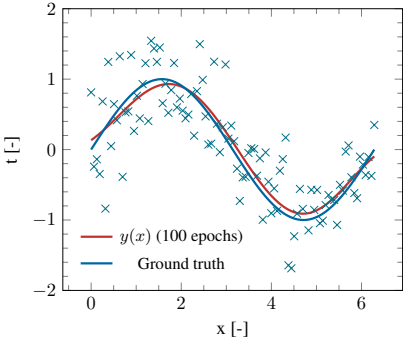
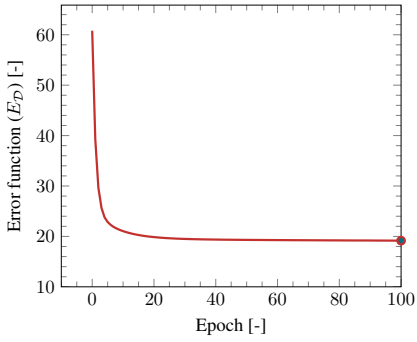
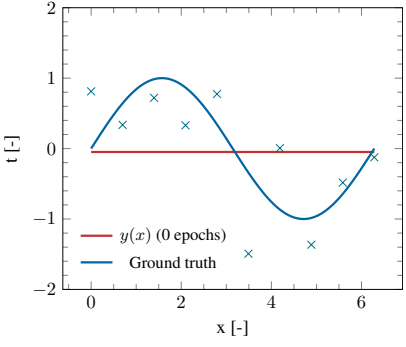


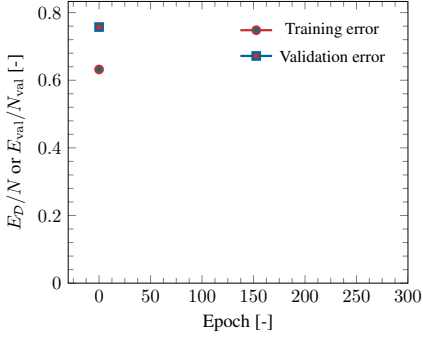


Stochastic Gradient Descent

Using SGD progress to spot signs of overfitting:

- Tracking the error on a validation dataset after every epoch
- This motivates the early stopping strategy popular in the deep learning community





Stochastic Gradient Descent

Using SGD progress to spot signs of overfitting:

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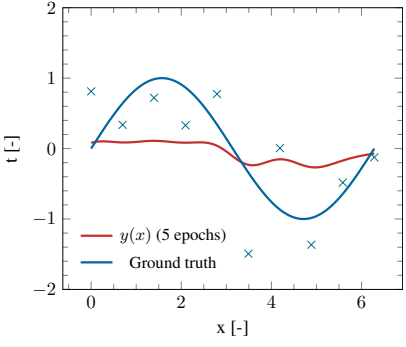

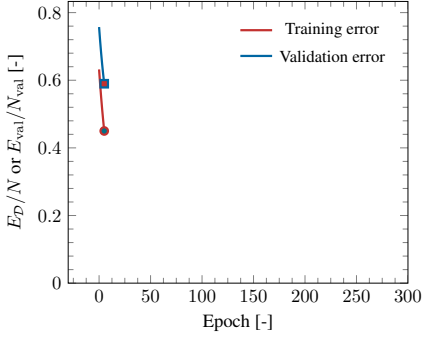

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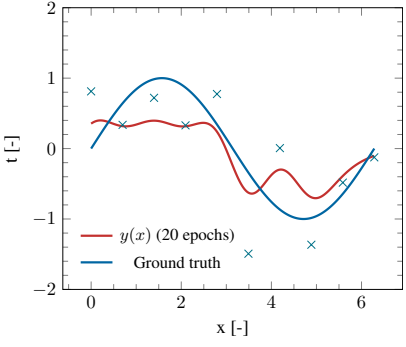

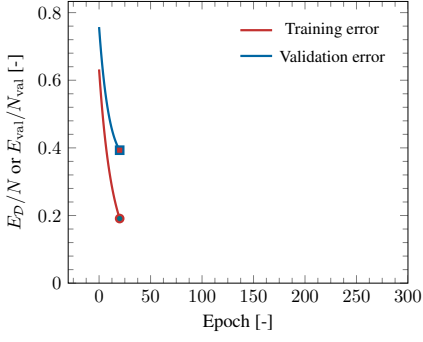

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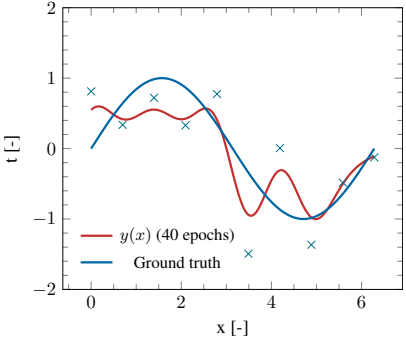

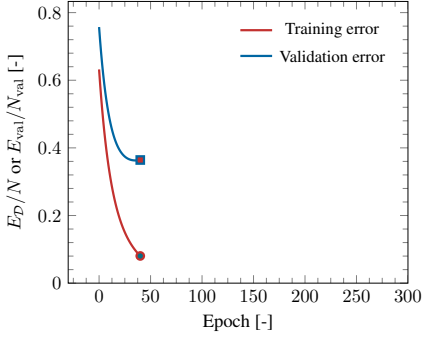

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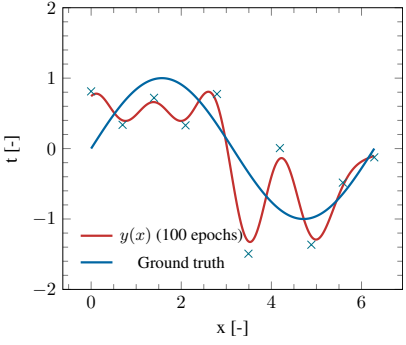

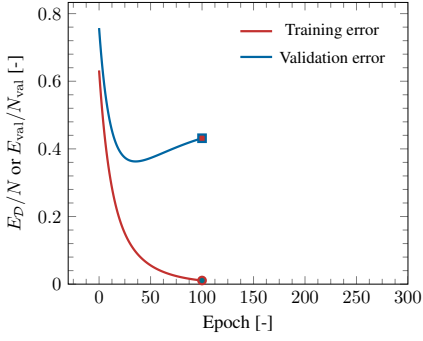

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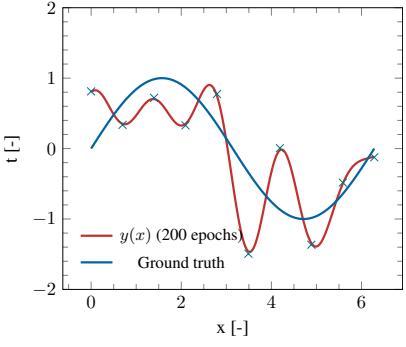

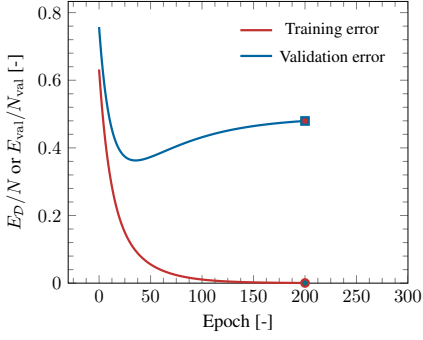

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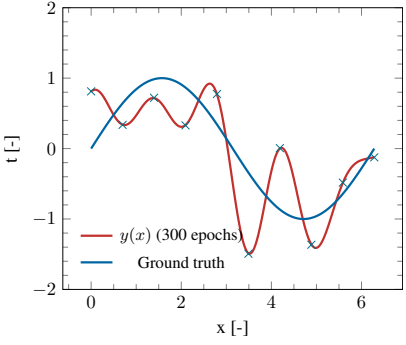
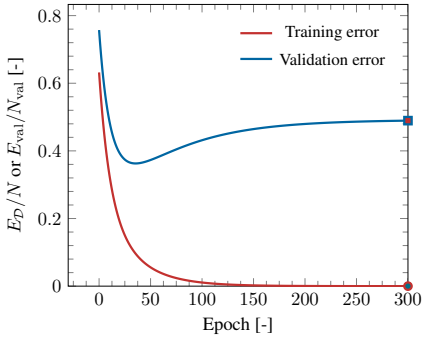


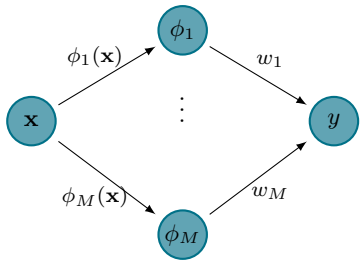


Adaptive basis functions

Up until now, the basis functions have been fixed a priori:

- Polynomials: number of terms M, polynomial degrees of each term
- Gaussians: bandwidth s, basis function centers μ_j

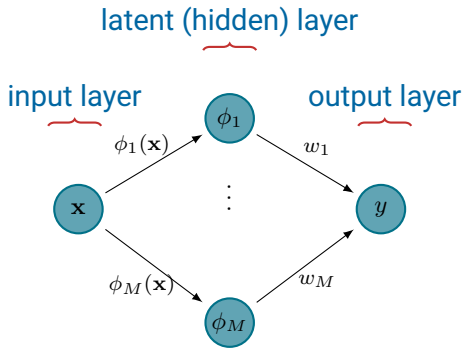
$$y = \phi_1(\mathbf{x})w_1 + \phi_2(\mathbf{x})w_2 + \cdots + \phi_M(\mathbf{x})w_M$$



Adaptive basis functions

For now, only half of the model is trainable:

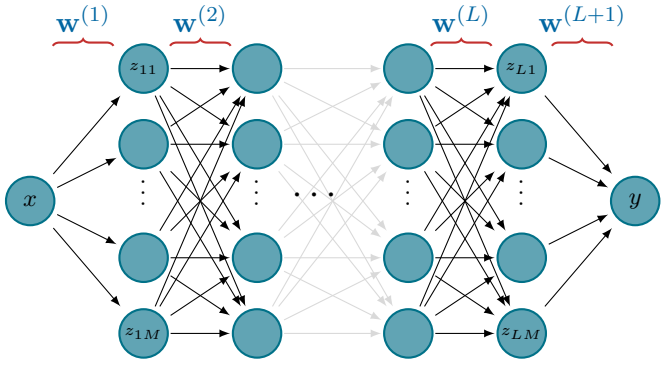
- Input to hidden encoding ($\phi_1 \cdots \phi_M$) fixed, hidden to output decoding ($\mathbf{w}$) trained
- What if we could also train the first half?



Artificial Neural Networks

Replacing basis functions by several layers of nonlinear transformations:

- Neural Network: layers of neurons linked by weighted synaptic connections
- Computing gradients becomes more complex, but all layers now have trainable weights



Neural Networks – Activation functions

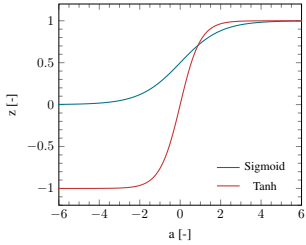
For a given neuron, forward propagation happens in two steps:

- A linear combination of values from the previous layer:

$$a_{lj} = \sum_{i}^{D} w_{ji}^{(l)} z_i^{(l-1)} + w_{j0}^{(l)}$$

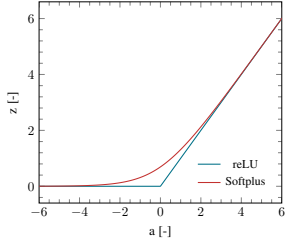
- A nonlinear transformation with an activation function:

$$z_{lj} = h\left(a_{lj}\right)$$



Choosing the activation function:

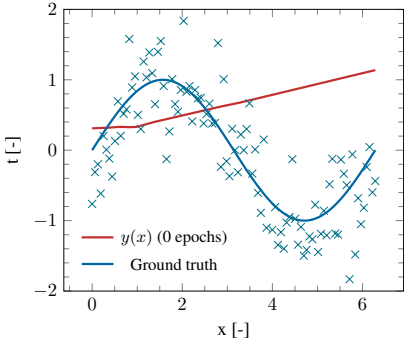
- Application dependent
- Can be seen as a hyperparameter

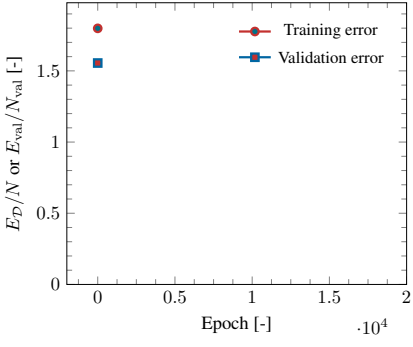


Neural Networks – Example

Same example as before, but now with a neural network:

- Full batch Adam SGD (variable learning rate)
- Two hidden layers, 10 neurons each, ReLU activation





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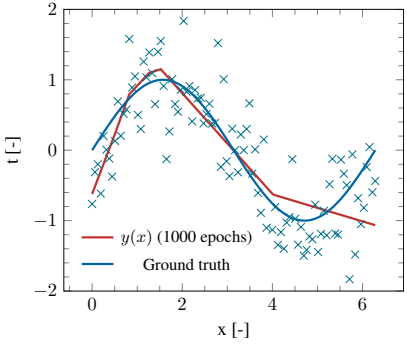

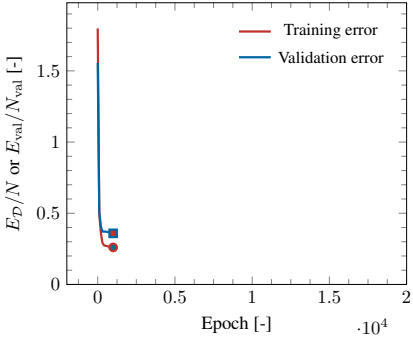

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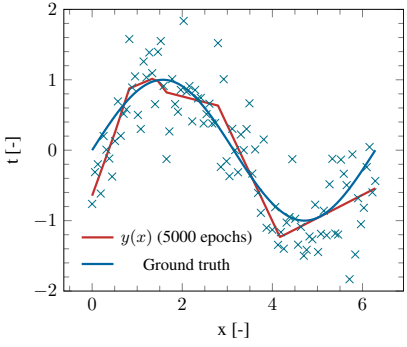

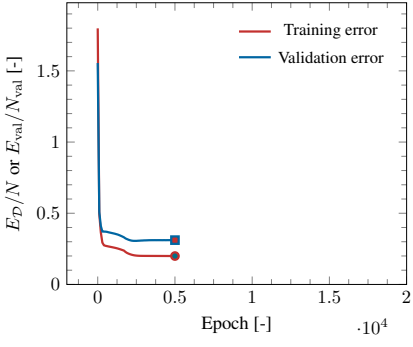

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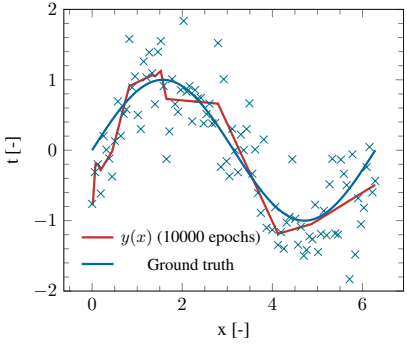

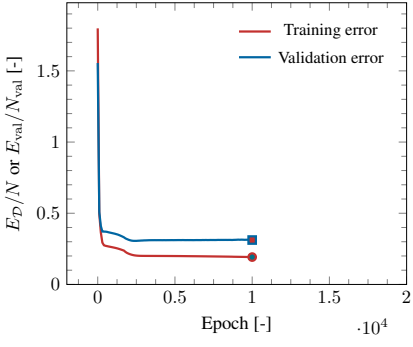

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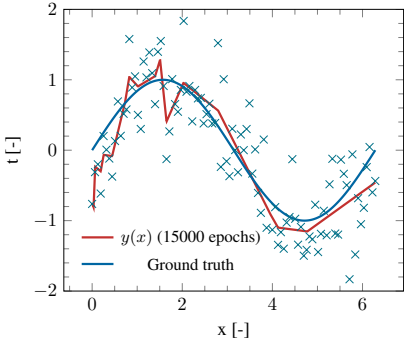

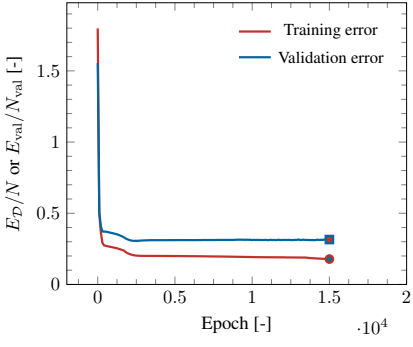

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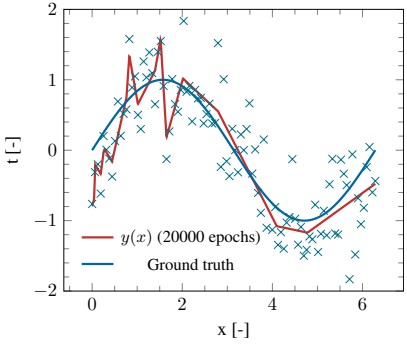
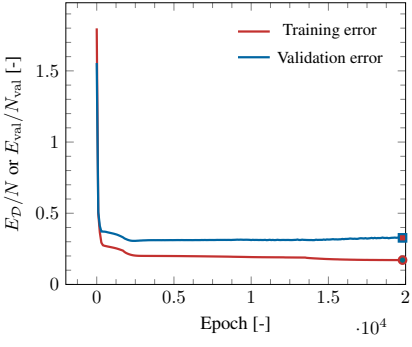




Break

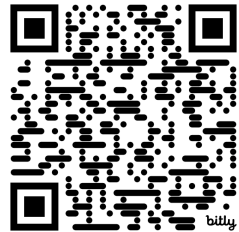
Let us take a 20-minute break

For later:

- Read the content in the book pages
- Play with a bunch of other interactive plots
- Look at Bayesian linear regression and try the exercises

Up next:

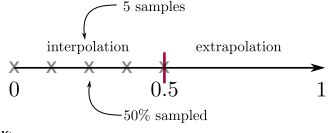
- The curse of dimensionality
- Breaking the curse — Bayesian ML and inductive biases
- Gaussian Processes for regression

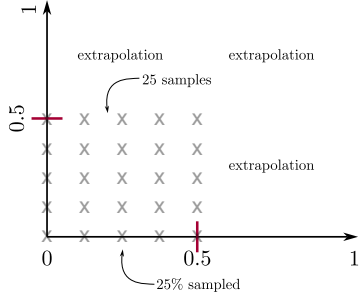


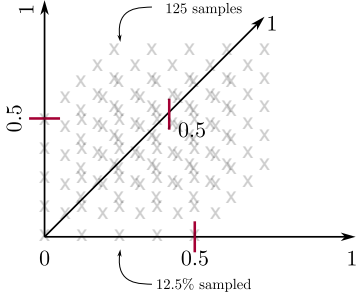
The Curse of Dimensionality

When building ML models, we rely on covering our feature space well enough. However...

- We need exponentially more samples to keep up as we go to higher dimensions







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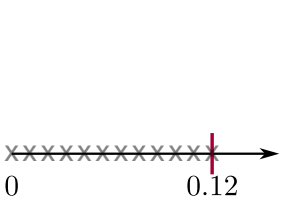
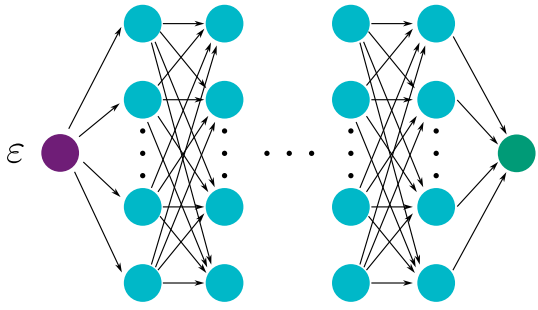
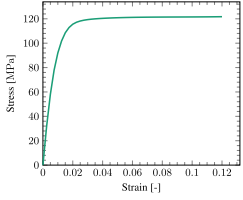
This is a huge issue for all sorts of tasks:

- From surrogate modeling to image processing







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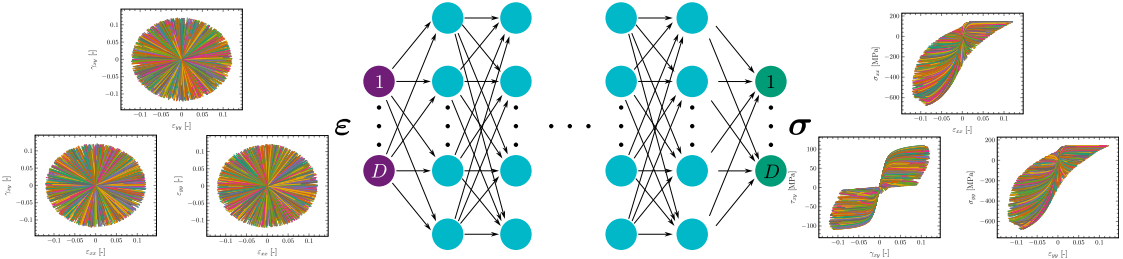

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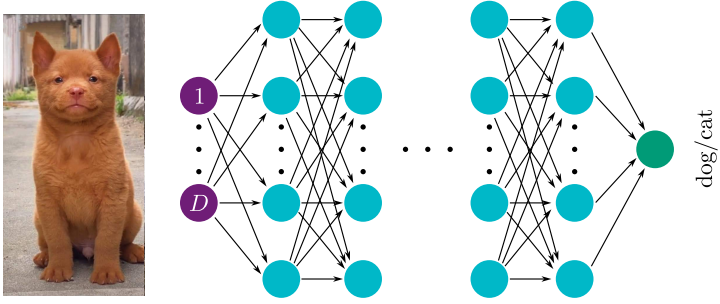
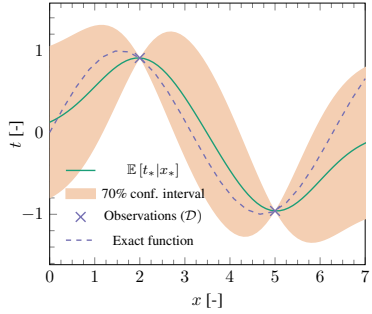


Breaking the curse

Bad news: fully breaking the curse is impossible. But with some extra tricks it can be alleviated:

- Introduce bias through prior beliefs ⇒ Bayesian ML (up next)
- Assume Euclidean or non-Euclidean spatial bias ⇒ Convolutional NNs, Graph NNs
- Explain patterns in lower dimensions with dimensionality reduction ⇒ PCA, Autoencoders
- Assume the data is explained by latent time dependencies ⇒ 1D CNNs, Recurrent NNs
- Introduce bias coming from physics knowledge ⇒ PINNs, hybrid models



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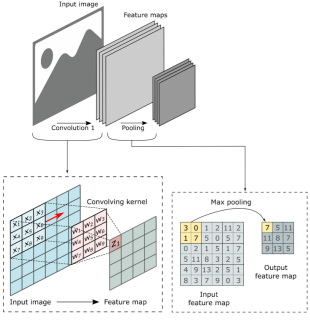

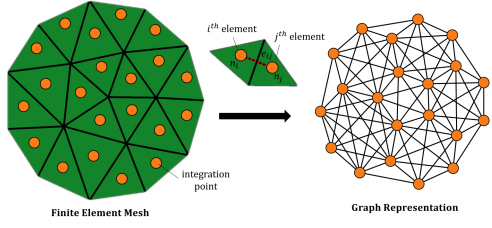

[Alzubaidi et al (2022), Rock Mech Rock Eng **55**:3719-3734]

[Vlassis and Sun (2022), arXiv:2208.00246v1]

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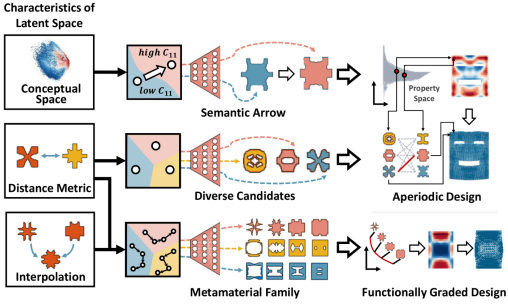

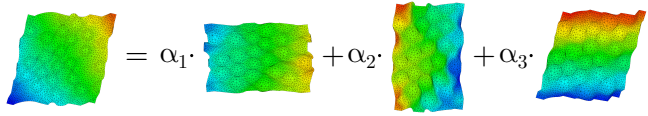

[Wang et al (2020), CMAME **372**:113377]

[Rocha et al (2019), CMAME **345**:644-670]

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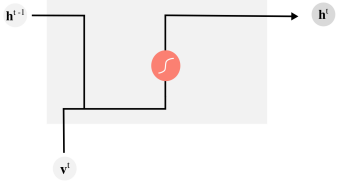
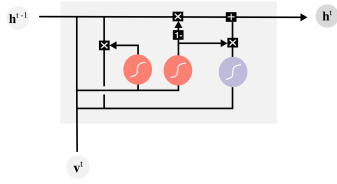
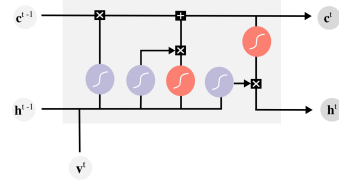


Classical RNN



Gated Recurrent Unit (GRU)



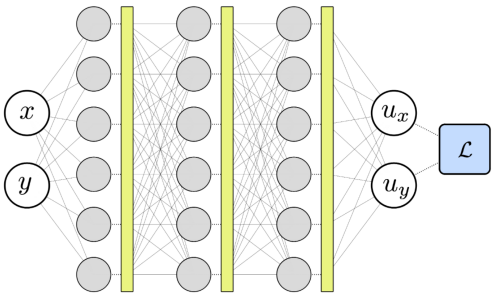
Long Short Term Memory (LSTM)

[Maia et al (2022), CMAME **407**:115934]

Breaking the curse

Bad news: fully breaking the curse is impossible. But with some extra tricks it can be alleviated:

- Introduce bias through prior beliefs ⇒ Bayesian ML (up next)
- Assume Euclidean or non-Euclidean spatial bias ⇒ Convolutional NNs, Graph NNs
- Explain patterns in lower dimensions with dimensionality reduction ⇒ PCA, Autoencoders
- Assume the data is explained by latent time dependencies ⇒ 1D CNNs, Recurrent NNs
- Introduce bias coming from physics knowledge ⇒ PINNs, hybrid models



[Haghighat et al (2020), arXiv:2003.02751v2]

$$\sigma_{ij,j} + f_i = 0$$
$$\sigma_{ij} = \lambda \delta_{ij} \varepsilon_{kk} + 2\mu \varepsilon_{ij}$$
$$\varepsilon_{ij} = \tfrac{1}{2}\left(u_{i,j} + u_{j,i}\right)$$
$$\mathcal{L} = |\sigma_{ij,j} + f_i|_\Omega$$

Collocation loss

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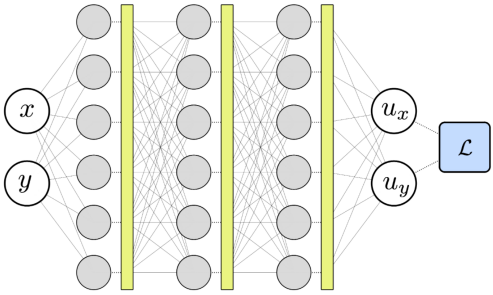

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Collocation loss — Dirichlet loss

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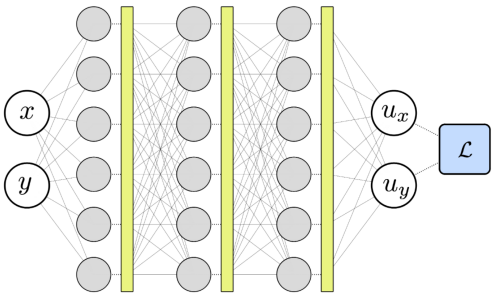

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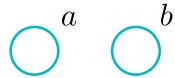
Collocation loss | Dirichlet loss | Neumann loss

Interlude — Probabilistic Graphs

Graphs with more than one variable imply a joint probability distribution:

- Two independent variables:



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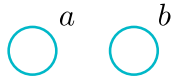
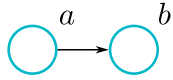
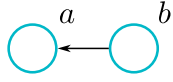


$$p(a, b) = p(a)p(b)$$

- We can use arrows to indicate dependency, causality or correlation through the Product Rule:



$$p(a, b) = p(a)p(b|a)$$



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Interlude — Bayes' Theorem

Consider a model with two variables x and y. We can use the Product Rule of probability to write:

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We can use Bayes' Theorem to model and update beliefs and uncertainties:

- The prior $p(y)$ expresses what we know about y before observing x
- The likelihood $p(x|y)$ models how much y can explain x
- The posterior $p(y|x)$ expresses how the knowledge about y changed after observing x

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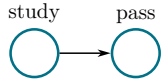
Bayes' Theorem states our willingness to change what we know about y after observing x:

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

Bayes' Theorem — Example

Let us consider a simple probabilistic model for predicting student performance:



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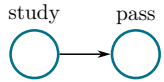

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Let us set some reasonable expectations:

$$p(S = 1) = 0.6 \qquad p(S = 0) = ?$$

$$p(P = 1|S = 1) = 0.9 \quad p(P = 1|S = 0) = 0.3$$

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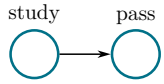

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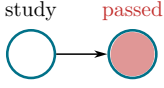
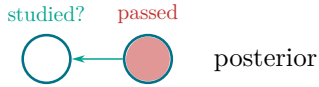
Now suppose we observe someone passed. How certain should we be that they studied?



observation

Bayes' Theorem — Example

Keeping our prior assumptions ignores important evidence. We use Bayes' Theorem instead:



$$p(S = 1|P = 1) = \frac{p(P = 1|S = 1)p(S = 1)}{p(P = 1)}$$

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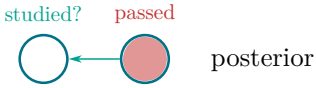

$$p(S=1|P=1) = \frac{p(P=1|S=1)p(S=1)}{p(P=1)}$$

$p(P=1,S) = p(S)p(P=1|S)$

Get together with someone and use the values below (10 minutes):

- Use the Sum Rule to compute the marginal $p(P=1)$ from the joint $P(P=1,S)$
- Use the values of $p(P=1|S=1)$ and $p(S=1)$ from below
- Put it all together above and compute the posterior $p(S=1|P=1)$

$$p(S=1) = 0.6 \qquad p(S=0) = 0.4$$

$$p(P=1|S=1) = 0.9 \quad p(P=1|S=0) = 0.3$$

$$p(P=0|S=1) = 0.1 \quad p(P=0|S=0) = 0.7$$

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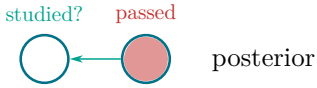

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How much did our knowledge shift? How does this compare to the prior? Does it make sense?

$$p(S = 1|P = 1) = \frac{0.9 \cdot 0.6}{0.9 \cdot 0.6 + 0.3 \cdot 0.4} = 0.818$$

Bayesian linear regression

Finally, let us use Bayes' Theorem properly and end up with a distribution for $\mathbf{w}$:

$$p(\mathbf{w}|\mathbf{t}) = \frac{p(\mathbf{t}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{t})} \quad \text{with} \quad p(\mathbf{w}) = \mathcal{N}\left(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}\right) \text{ and } p(\mathbf{t}|\mathbf{w}) = \mathcal{N}\left(\mathbf{t}|\mathbf{\Phi}\mathbf{w}, \beta^{-1}\mathbf{I}\right)$$

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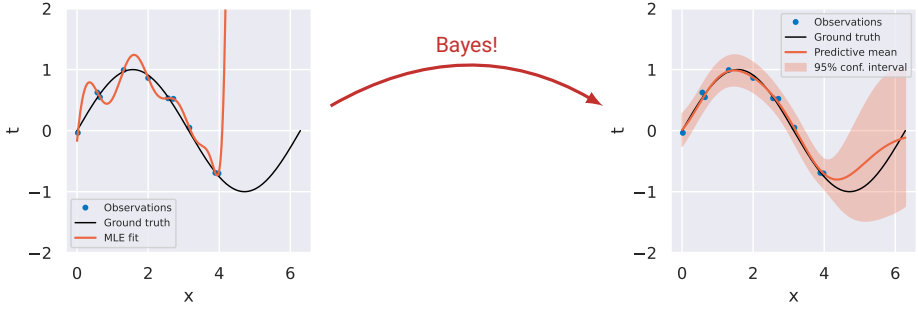
The result takes the simple form:

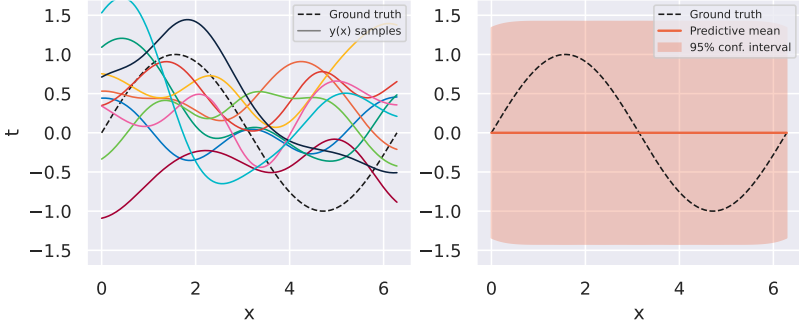
$$p(\mathbf{w}|\mathbf{t}) = \mathcal{N}\left(\mathbf{w}|\mathbf{m}, \mathbf{S}\right) \quad \text{with} \quad \mathbf{m} = \beta\mathbf{S}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t} \text{ and } \mathbf{S}^{-1} = \alpha\mathbf{I} + \beta\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}$$



Sampling models from the posterior

Since $\mathbf{w}$ is probabilistic, we have a bag of models at our disposal:

- Take a sample $\widetilde{\mathbf{w}}$ from $\mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I})$
- Compute $y(\mathbf{x}, \widetilde{\mathbf{w}})$ for our whole range of $\mathbf{x}$



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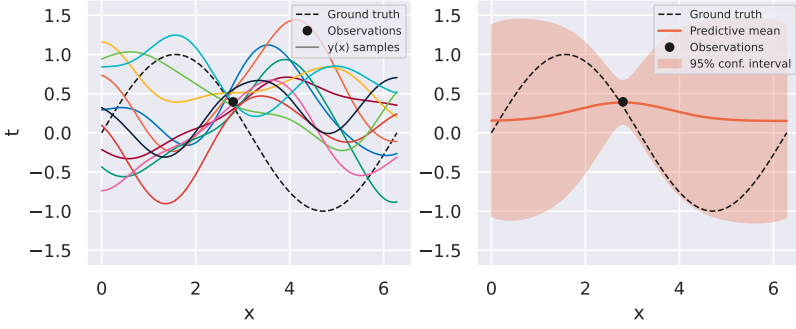

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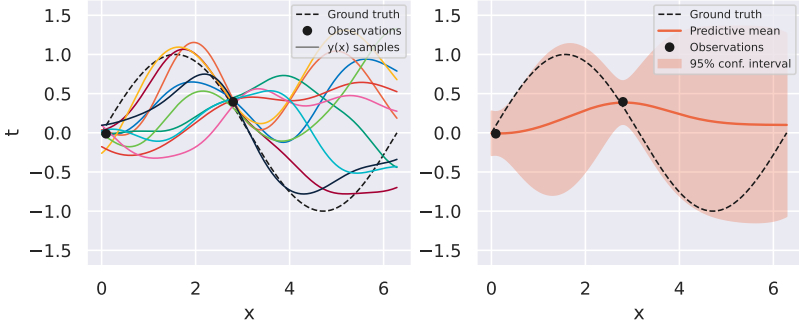

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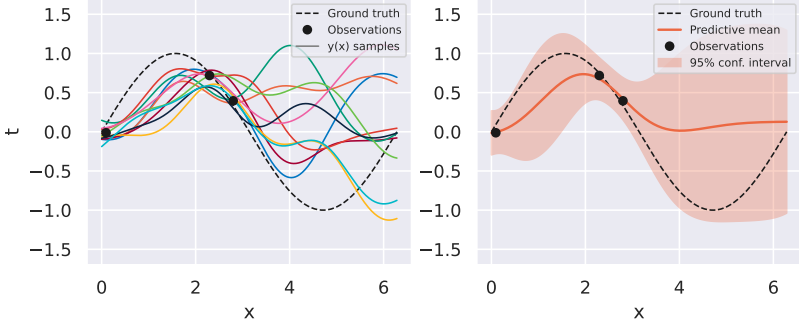

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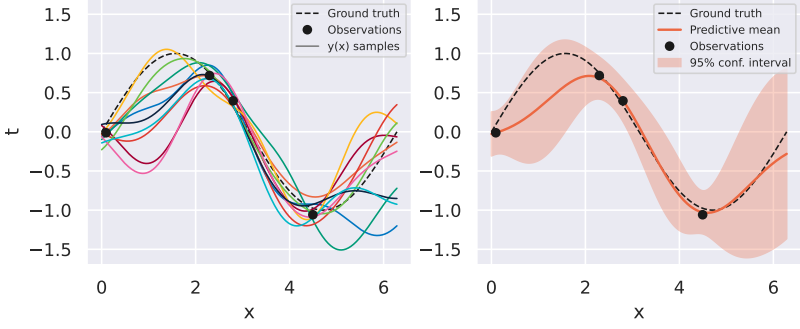

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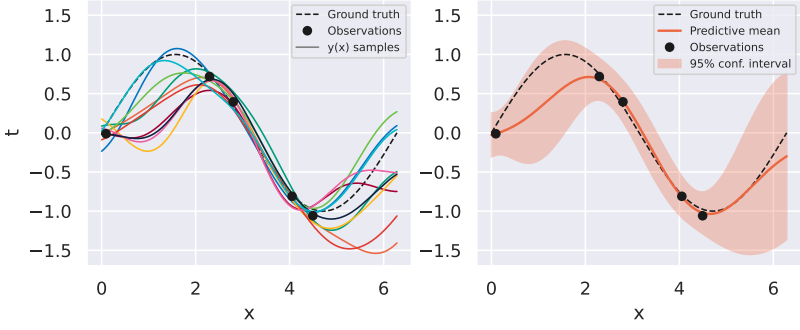

From weights to functions

Now we gather all values of y for a single realization of $\mathbf{w}$ into a vector:

$$\mathbf{y} = \mathbf{\Phi}\mathbf{w} \quad \text{with} \quad \mathbf{\Phi}_{nk} = \phi_k(\mathbf{x}_n)$$

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Because $\mathbf{\Phi}$ is a linear deterministic operator, $\mathbf{y}$ is also Gaussian:

$$p(\mathbf{y}) = \mathcal{N}\left(\mathbf{y}|\mathbf{0}, \alpha^{-1}\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}\right)$$

- Note that $\mathbf{w}$ is now gone. This is now officially a non-parametric model!
- Instead of sampling from $p(\mathbf{w})$, we can now sample models from $p(\mathbf{y})$

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We can write the above in a more compact way:

- Define a kernel that relates two values of $\mathbf{x}$ and returns a scalar:

$$k(\mathbf{x}, \mathbf{x}') = \frac{1}{\alpha}\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}')$$

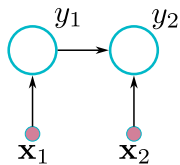
- Express $p(\mathbf{y})$ in terms of the kernel:

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}) \quad \text{with} \quad K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

From weights to functions

As always, we can represent this model with a graph

- Starting with just a few variables



$$p(y_1, y_2) = \mathcal{N}\left(\mathbf{y}_{12} \mid \begin{bmatrix} m(\mathbf{x}_1) \\ m(\mathbf{x}_2) \end{bmatrix}, \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) \end{bmatrix}\right) \equiv \mathcal{N}\left(\mathbf{y}_{12} \mid \mathbf{m}_{12}, \mathbf{K}_{12}\right)$$

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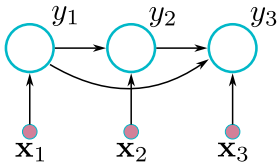

$$p(\mathbf{y}_{12}, y_3) = \mathcal{N}\left(\mathbf{y}_{123} \mid \begin{bmatrix}\mathbf{m}_{12}\\ m(\mathbf{x}_3)\end{bmatrix}, \begin{bmatrix}\mathbf{K}_{12} & k(\mathbf{x}_1,\mathbf{x}_3)\\ & k(\mathbf{x}_2,\mathbf{x}_3)\\ k(\mathbf{x}_3,\mathbf{x}_1) \quad k(\mathbf{x}_3,\mathbf{x}_2) & k(\mathbf{x}_3,\mathbf{x}_3)\end{bmatrix}\right) \equiv \mathcal{N}\left(\mathbf{y}_{123} \mid \mathbf{m}_{123}, \mathbf{K}_{123}\right)$$

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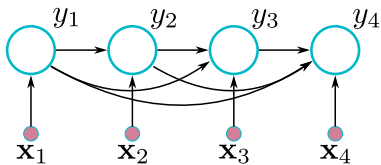
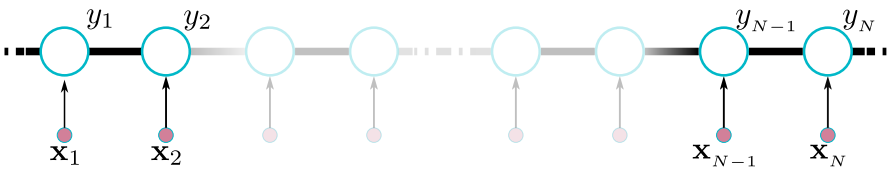


$$p(\mathbf{y}_{123}, y_4) = \mathcal{N}\left(\mathbf{y}_{1234} \mid \begin{bmatrix}\mathbf{m}_{123} \\ m(\mathbf{x}_4)\end{bmatrix}, \begin{bmatrix} & \mathbf{K}_{123} & & k(\mathbf{x}_1, \mathbf{x}_4) \\ & & & k(\mathbf{x}_2, \mathbf{x}_4) \\ & & & k(\mathbf{x}_3, \mathbf{x}_4) \\ k(\mathbf{x}_4, \mathbf{x}_1) & k(\mathbf{x}_4, \mathbf{x}_2) & k(\mathbf{x}_4, \mathbf{x}_3) & k(\mathbf{x}_4, \mathbf{x}_4) \end{bmatrix}\right) \equiv \mathcal{N}\left(\mathbf{y}_{1234} \mid \mathbf{m}_{1234}, \mathbf{K}_{1234}\right)$$

From weights to functions

As always, we can represent this model with a graph

- Starting with just a few variables
- We can generalize this for any number of nodes. Assuming zero mean:

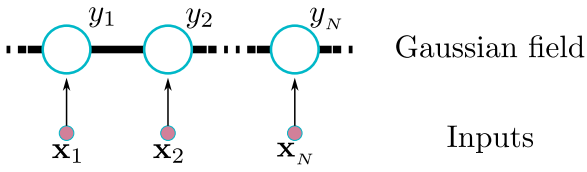


$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K})$$

From weights to functions

As always, we can represent this model with a graph

- Starting with just a few variables
- We can generalize this for any number of nodes. Assuming zero mean
- Finally, we can use a more compact version:



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A GP is fully described by a mean function and a covariance kernel:

$$y(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')\right)$$

- The kernel dictates the correlation between function values
- Edge case: $k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \delta(\mathbf{x} - \mathbf{x}') \Rightarrow \mathbf{K} = \sigma_f^2 \mathbf{I}$ (white noise random walk)

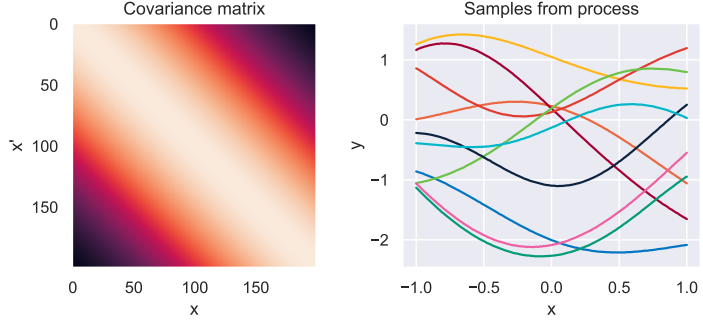
Kernel engineering — squared exponential

A very popular kernel in many applications, powerful and flexible:

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2}\right)$$

- Hyperparameters: process variance σ_f^2, length scale ℓ
- Equivalent to an RBF kernel with infinite (!) basis functions

process variance $\sigma_f^2 = 1$, length scale $\ell = 1$



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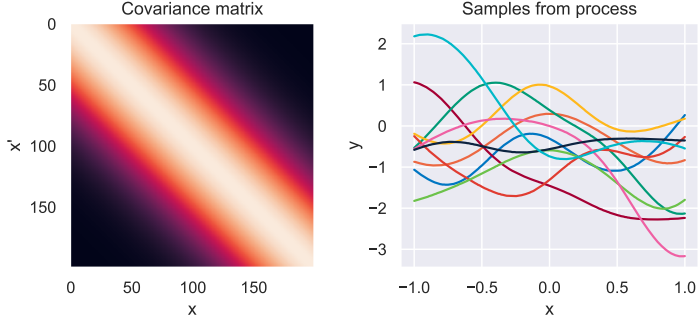

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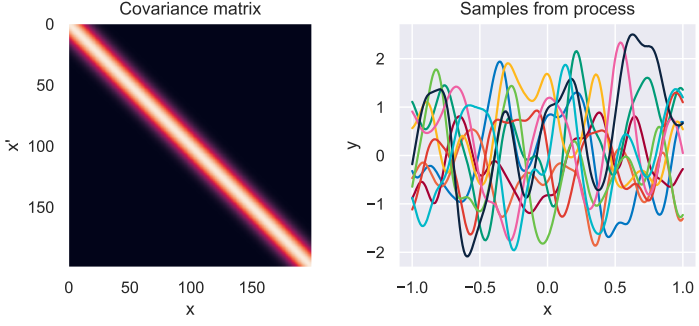


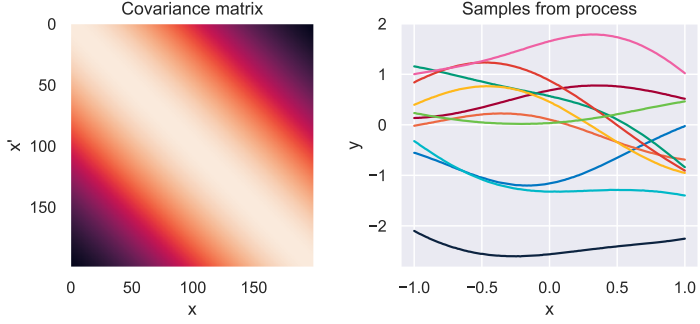
Kernel engineering — Matérn

A kernel for when differentiability is an issue:

$$k(\mathbf{x}, \mathbf{x}') = \frac{\sigma_f^2}{\Gamma(\nu)2^{\nu-1}} \left(\frac{\sqrt{2\nu}}{\ell} \|\mathbf{x} - \mathbf{x}'\| \right)^{\nu} K_\nu \left(\frac{\sqrt{2\nu}}{\ell} \|\mathbf{x} - \mathbf{x}'\| \right)$$

- Hyperparameters: process variance σ_f^2, length scale ℓ, differentiability parameter ν

$\nu \to \infty$ (infinitely differentiable)



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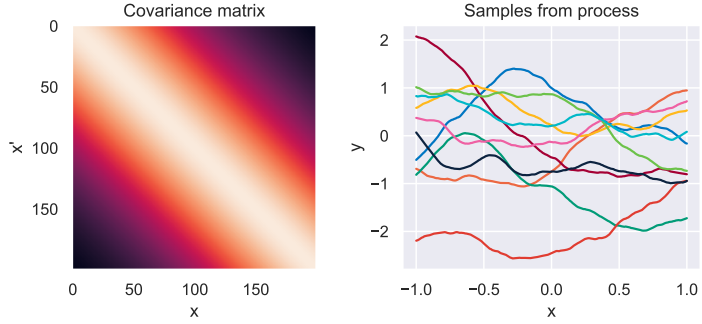

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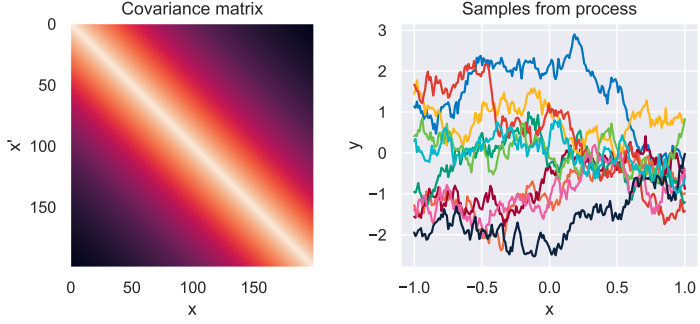

Gaussian processes for regression

For regression, we need to observe some targets and predict for new inputs

- Assume targets are Gaussian-distributed around $y(\mathbf{x})$:

$$p(t|y) = \mathcal{N}\left(t|y(\mathbf{x}), \beta^{-1}\right)$$

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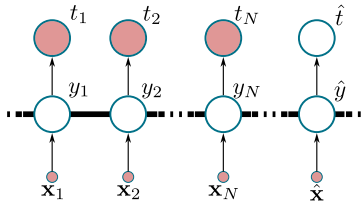

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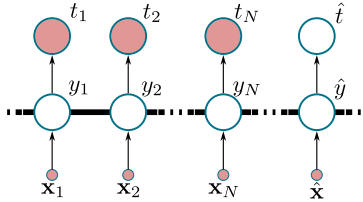

- From the standard expressions for the Gaussian, we have a marginal over the targets:

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y})\,\mathrm{d}\mathbf{y} = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, K(\mathbf{X},\mathbf{X}) + \beta^{-1}\mathbf{I}\right)$$

GPs for regression — joint distribution

How to make new predictions? We need a joint between $\mathbf{t}$ and $\hat{t}$:

$$p(\mathbf{t}, \hat{t}) = \mathcal{N}\left(\mathbf{t}, \hat{t} \mid \mathbf{0}, \begin{bmatrix} K(\mathbf{X}, \mathbf{X}) + \beta^{-1}\mathbf{I} & K(\mathbf{X}, \hat{\mathbf{x}}) \\ K(\hat{\mathbf{x}}, \mathbf{X}) & k(\hat{\mathbf{x}}, \hat{\mathbf{x}}) + \beta^{-1} \end{bmatrix}\right)$$

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Note the meaning and sizes of these submatrices:

- $K(\mathbf{X}, \mathbf{X}) + \beta^{-1}\mathbf{I}$: Correlation between training inputs, with added observation noise ($N \times N$)
- $K(\mathbf{X}, \hat{\mathbf{x}})$: Correlation between training targets and the new target ($N \times 1$)
- $K(\hat{\mathbf{x}}, \mathbf{X})$: Correlation between the new target and training targets ($1 \times N$)
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Note that we are predicting a single new value at $\hat{\mathbf{x}}$

- What would be the sizes of these matrices if we were predicting at 1000 new locations?

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But given that we already have a joint Gaussian, we can just use our old conditioning expressions:

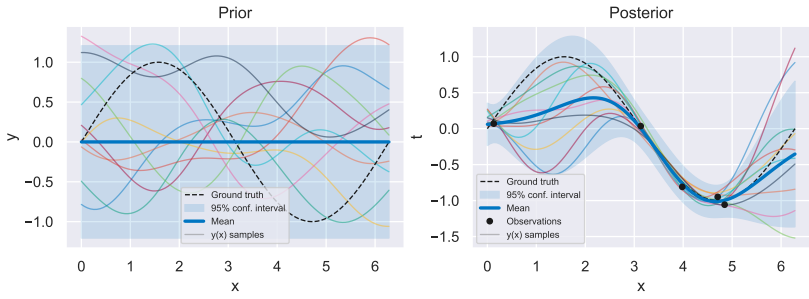
$$p(\hat{t}|\mathbf{t}) = \mathcal{N}\left(\hat{t}|\hat{m}, \hat{\sigma}^2\right)$$

$$\hat{m} = K\left(\hat{\mathbf{x}}, \mathbf{X}\right)\left[K\left(\mathbf{X}, \mathbf{X}\right) + \beta^{-1}\mathbf{I}\right]^{-1}\mathbf{t}$$

$$\hat{\sigma}^2 = k\left(\hat{\mathbf{x}}, \hat{\mathbf{x}}\right) - K\left(\hat{\mathbf{x}}, \mathbf{X}\right)\left[K\left(\mathbf{X}, \mathbf{X}\right) + \beta^{-1}\mathbf{I}\right]^{-1}K\left(\mathbf{X}, \hat{\mathbf{x}}\right) + \beta^{-1}$$

GPs for regression — example

Let us go back to our running sine-wave example. We observe $N = 5$ data points with a SE GP:



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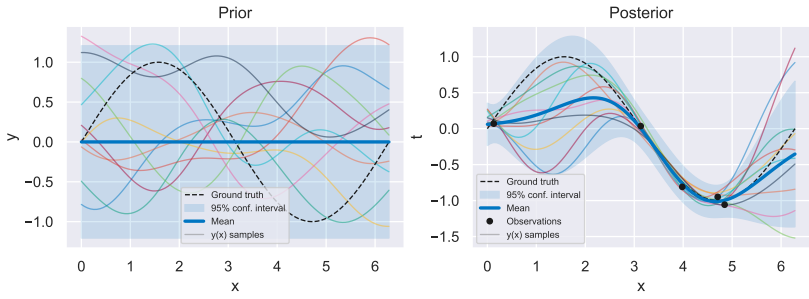

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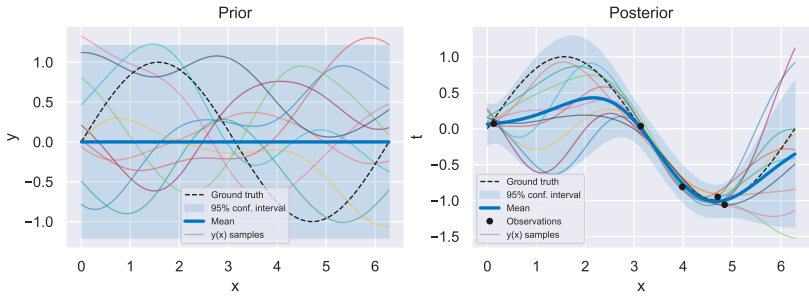

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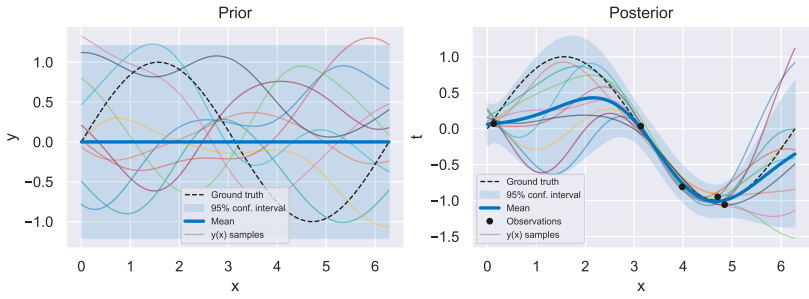

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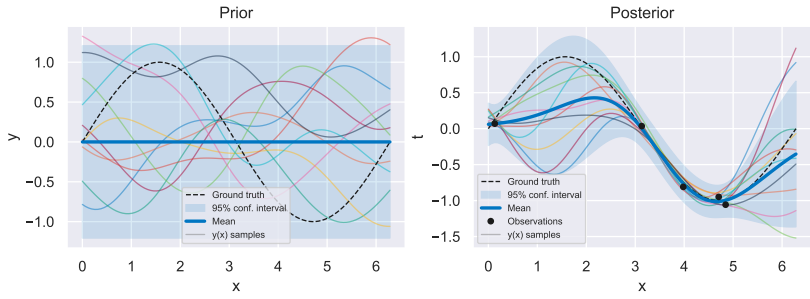

- We have a prior and a posterior process, we can sample from both
- All posterior samples pass close to the observations (this closeness is proportional to β)
- Away from data the samples spread out and the variance increases
- The model avoids overfitting even for this very small dataset

Learning and model selection

Hyperparameters can be learned without a validation set!

- We look at the marginal likelihood, which is quite easy in this case:

$$p(\mathbf{t}) = \mathcal{N}\left(\mathbf{t}|\mathbf{0}, K(\mathbf{X}, \mathbf{X}) + \beta^{-1}\mathbf{I}\right)$$

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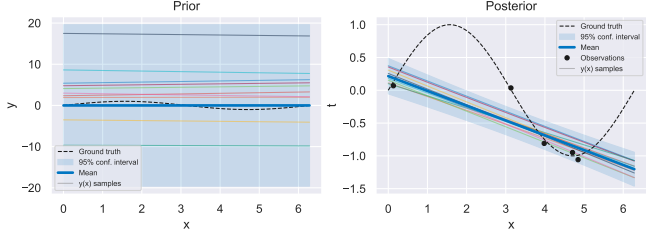

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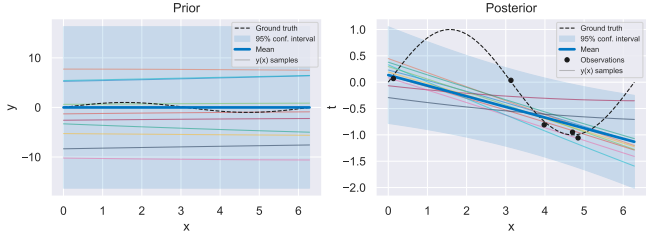

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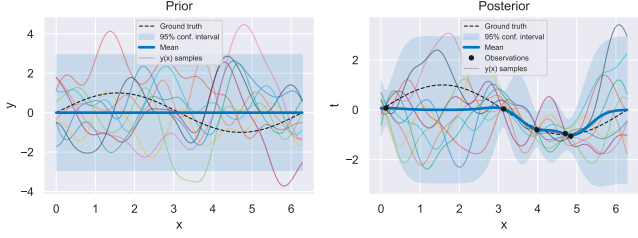

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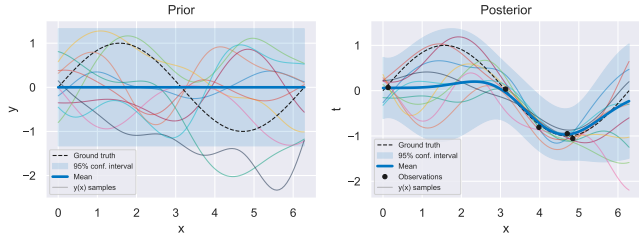

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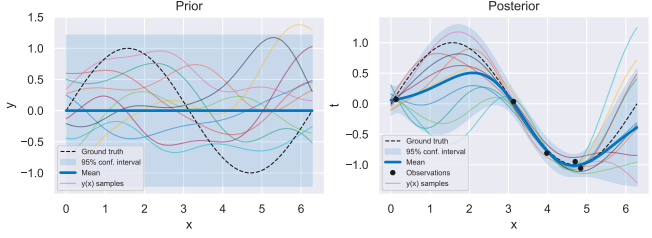

End of this part

Key takeaways:

- ML inherits much of its foundation from statistics
- Bias/variance tradeoff is an everyday struggle
- Bayesian ML can lead to very robust models
- Nevertheless, high-dimensional feature spaces require clever solutions

Up next:

- Introducing physics-based bias to ML models
- Structural bias through operator architectures
- Regression with ML across the scales

We hope you enjoyed this part!