Regression models

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Outline

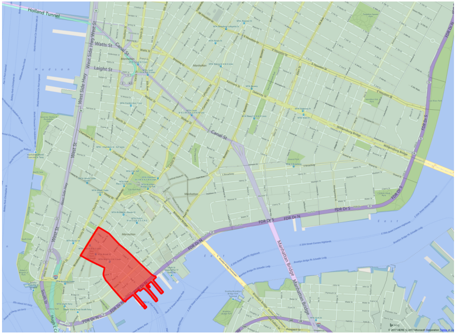
- Case study: Modeling taxi demand in NYC
- Linear regression
- Poisson regression
- Heteroscedastic regression

Modeling taxi demand in New York City

- (Almost) all taxi trips in NYC from 2009 to mid 2016
- Original files have one trip per line
  - Pick-up location and time
  - Drop-off location and time
  - Other variables such as trip price and number of passengers
- Weather data from the National Oceanic and Atmospheric Administration
- Research question: **model taxi pickups across the city**
- Useful to optimize taxi service
  - Similar to many other demand problems (shared modes, public transport, energy, water, goods, communication...)

Modeling taxi demand in New York City (cont'd)

- Preprocessed data
  - Grouped data by census tract in 1 hour intervals
  - Extended grouped taxi data with relevant weather information
- Case study: **Wall Street**



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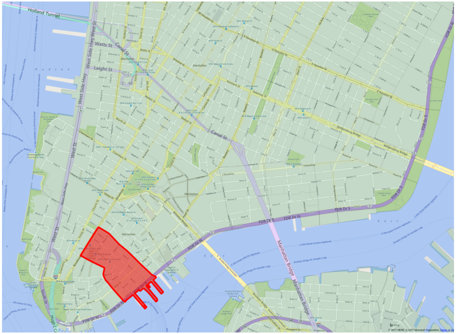
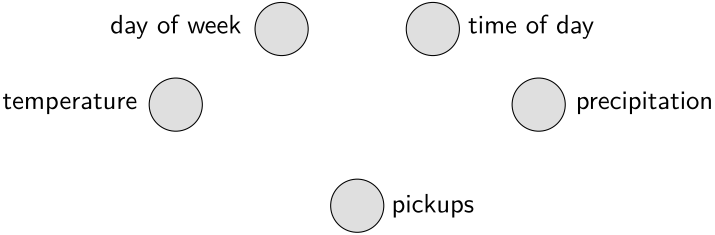


- What we know: day of the week, time of the day, temperature, precipitation, etc.
- Target variable: number of taxi pickups

Modeling taxi demand in New York City (cont'd)

- Let's start thinking about the graphical model...



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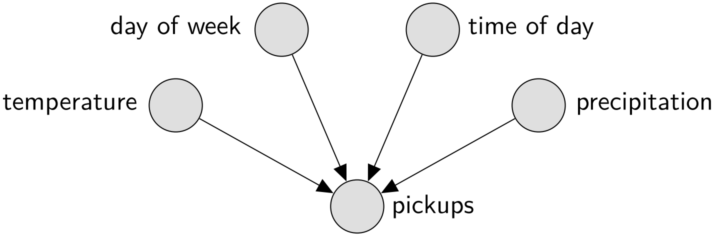

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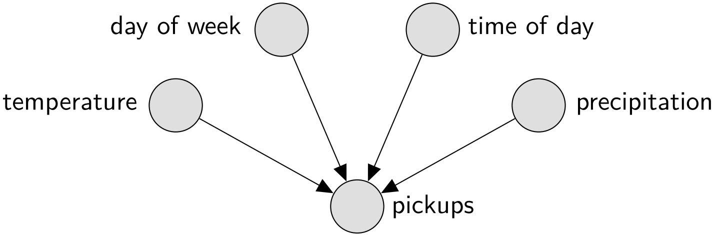

- What distribution should we assign to the pickups variable?
- How should we model the dependency of the pickups on the other variables?
- Do we need to assign distributions to these other variables (i.e. temperature, day of week, time of day, etc.)?
- This puts us right into the **regression** framework!

Regression

- Regression - predict response variable y from a collection of D predictor variables $x_1, x_2, \ldots, x_d, \ldots, x_D$

  y - target, response or dependent variable
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- A few examples:
  - travel time prediction
  - predicting demand for autonomous vehicles
  - temperature/rainfall forecast
  - estimation of audience to a concert
  - prediction of future values of a share or a commodity (e.g. petrol)
  - prediction of house prices, number of voters in a state, births in a year
  - and, of course, predicting taxi demand!

Linear regression

- The dependent variable y is a function of all the predictor variables

$$y = f(x_1, x_2, \ldots, x_d, \ldots, x_D)$$

- Ok, but what function?
- Simplest approach is to assume a **linear relationship**

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_D x_D = \beta_0 + \sum_{d=1}^{D} \beta_d x_d$$

β_0 is the *intercept* (or bias) and $\{\beta_1, \beta_2, \ldots, \beta_D\}$ are the *coefficients* (or weights)

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- We can write this more compactly using **vector notation**

$$y = \beta_0 + \boldsymbol{\beta}^\mathsf{T} \mathbf{x}$$

  where $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_D)^\mathsf{T}$ and $\mathbf{x} = (x_1, x_2, \ldots, x_D)^\mathsf{T}$

Note

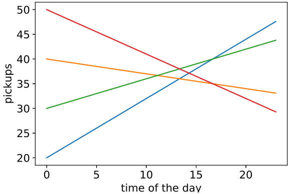
The intercept β_0 can be seen as a coefficient for a special covariate x_0 that is always equal to 1. Thus, it is sometimes omitted.

Linear regression

- Linear assumption can seem naive...

$$y = f(\mathbf{x}) = \boldsymbol{\beta}^\mathsf{T}\mathbf{x}$$

- But, the features $\mathbf{x}$ can be extremely **flexible**!



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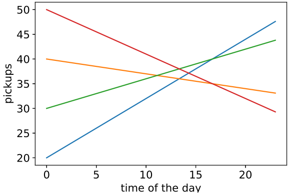

- But, the features $\mathbf{x}$ can be extremely **flexible**!
  - Any characteristic of the data
  - Indicator functions and 1-of-K encodings (e.g. $x_1 = \mathbb{I}[\text{weekend} = \text{True}]$)
  - Transformations of the original features (e.g. $x_2 = \log x_1$)
  - Basis expansion (e.g. $x_2 = x_1^2$ and $x_3 = x_1^3$) - polynomial fitting!
  - Interactions between features (e.g. $x_3 = x_1 x_2$)

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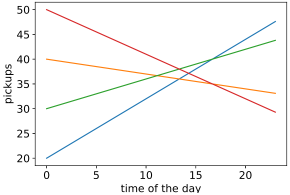

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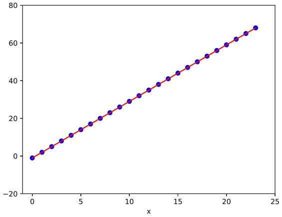
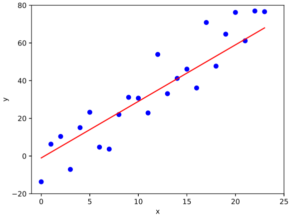
- Key aspects of linear regression
  - Simplicity
  - Flexibility
- One of the most important and widely used methods in statistics and machine learning!

Linear regression

- In practice observations are **noisy**



(a) dream world



(b) tough reality

- Add error term ϵ to account for observation noise

$$y = \boldsymbol{\beta}^{\mathsf{T}}\mathbf{x} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- We can equivalently write

$$\mathcal{N}(y|\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}, \sigma^2)$$

Linear regression as a graphical model

- We have a dataset $\mathcal{D}$ consisting of N observations of the targets y_n which depend on their corresponding explanatory variables $\mathbf{x}_n$

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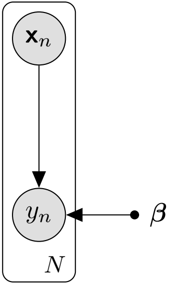

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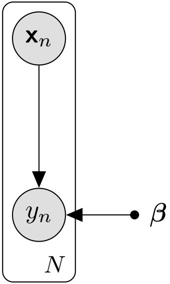

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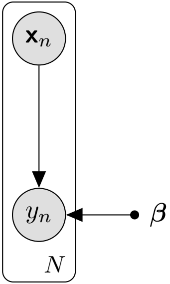

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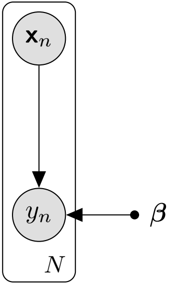

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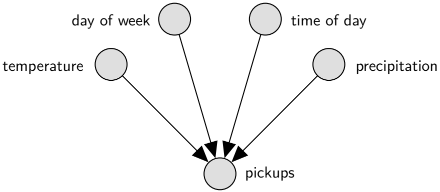
Note

We don't care about modeling $p(\mathbf{y}, \mathbf{X}, \beta, \sigma)$. This is called a **conditional model** and contrasts with fully generative models.

Going back to our taxi demand case study...

- Let's revise the **modeling assumptions** that we made



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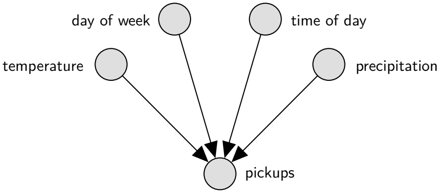

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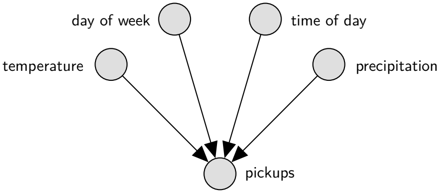

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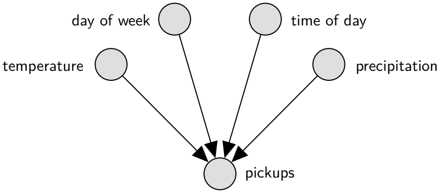

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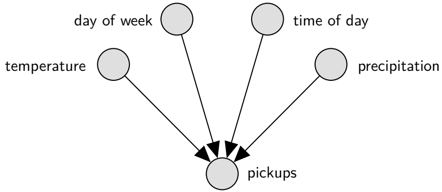

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  - In this case, no. They are always observed and we are only interested in modeling the behavior of the pickups variable

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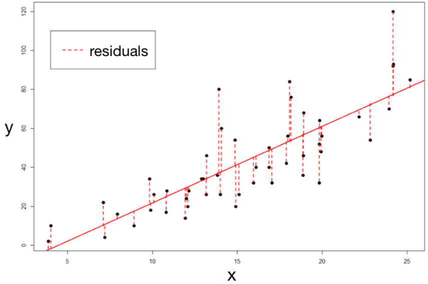
$$\hat{\beta} = \arg\min_{\boldsymbol{\beta}} \sum_{n=1}^{N} \left(y_n - \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n\right)^2$$



- Has a nice analytical solution (the famous *normal equation*)

$$\hat{\beta} = (\mathbf{X}^\mathsf{T}\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

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Don't believe it?

Replace $\mathcal{N}(y_n|\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}_n, \sigma^2)$ in the expression above by the definition of the Gaussian, take the derivative w.r.t. $\boldsymbol{\beta}$, set it to zero and solve for $\boldsymbol{\beta}$.

- This is called **maximum likelihood estimation (MLE)**!
- It allows to find a **point estimate** for the parameters in a probabilistic model

Adding priors

- We have been assuming the coefficients β to be deterministic values, but...
  - What if we have some prior knowledge on the values of β?
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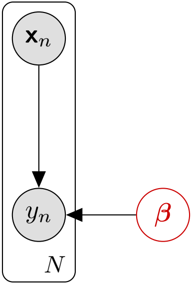
- This encourages the values of β to be centered around zero with more or less variance depending on λ
  - Larger λ leads to more **overfit**
  - Smaler λ leads to more **underfit**

Bayesian linear regression model

- Updated graphical model



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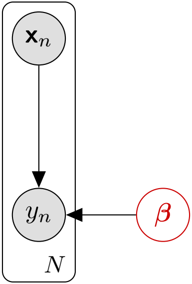

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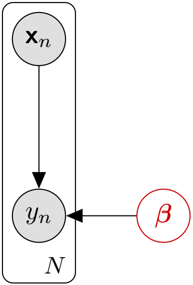

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- Joint probability distribution now factorizes as

$$p(\mathbf{y}, \boldsymbol{\beta}|\mathbf{X}, \sigma, \lambda) = p(\boldsymbol{\beta}|\lambda) \prod_{n=1}^{N} p(y_n|\boldsymbol{\beta}, \mathbf{x}_n, \sigma)$$

$$= \underbrace{\mathcal{N}(\boldsymbol{\beta}|\mathbf{0}, \lambda\mathbf{I})}_{\text{prior}} \times \underbrace{\prod_{n=1}^{N} \mathcal{N}(y_n|\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n, \sigma^2)}_{\text{likelihood}}$$

Inference

- **Goal:** compute **posterior** distribution on β
- Following Bayes' theorem

$$\underbrace{p(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}, \sigma, \lambda)}_{\text{posterior}} \propto \underbrace{\mathcal{N}(\boldsymbol{\beta}|\mathbf{0}, \lambda\mathbf{I})}_{\text{prior}} \times \underbrace{\prod_{n=1}^{N} \mathcal{N}(y_n|\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}_n, \sigma^2)}_{\text{likelihood}}$$

- We can find an analytical solution to this - exact inference is possible!
- We will cover inference methods later in the course...
- For now, Stan will take care of it for us :-)

Model estimation: MAP

- Alternatively to computing the posterior distribution on $\boldsymbol{\beta}$, we can find a point estimate by maximizing the (log) joint probability of the model

$$\hat{\boldsymbol{\beta}} = \arg\max_{\boldsymbol{\beta}} \log \left(\mathcal{N}(\boldsymbol{\beta}|\mathbf{0}, \lambda \mathbf{I}) \prod_{n=1}^{N} \mathcal{N}(y_n|\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n, \sigma^2) \right)$$

$$= \arg\max_{\boldsymbol{\beta}} \left(\log \mathcal{N}(\boldsymbol{\beta}|\mathbf{0}, \lambda \mathbf{I}) + \sum_{n=1}^{N} \log \mathcal{N}(y_n|\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n, \sigma^2) \right)$$

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- This is called **maximum-a-posteriori (MAP)** estimation

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Note

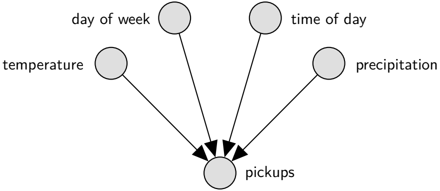
This is just like the MLE estimator plus a new term: $\log \mathcal{N}(\boldsymbol{\beta}|\mathbf{0}, \lambda\mathbf{I})$. It penalizes the coefficients $\boldsymbol{\beta}$ for getting too large (overfitting). This is called **regularization**.

Playtime!

- Ancestral sampling from linear regression model
  - See “05 - Regression models - Part 1.ipynb" notebook
  - Expected duration: 15 minutes
- Linear regression model of taxi pickups in NYC
  - See “05 - Regression models - Part 2.ipynb" notebook
  - Do section 2.1
  - Expected duration: 1 hour

Going back to our taxi demand case study...

- Let's revise (again) the **modeling assumptions** that we made



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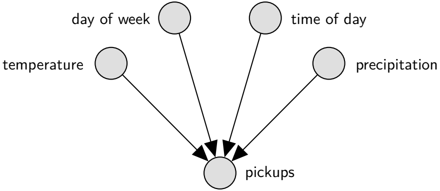

- What distribution should we assign to the pickups variable?
    - Gaussian
- But is this really the most appropriate distribution in this case?
    - Number of pickups is a count: $y_n \in \mathbb{N}$
    - A common distribution for modelling count data is the **Poisson**

Poisson regression

- “Poisson distribution expresses the probability of a given number of events occurring in a fixed interval of time and/or space if these events occur with a **known constant rate** and independently of the time since the last event"

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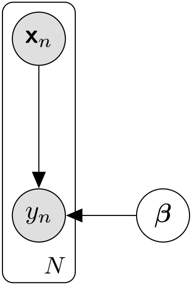
Note

Link functions get their names from the inverse of the transformation.

Bayesian poisson regression model

- Graphical model looks the same as before



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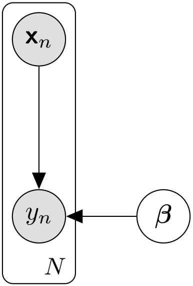

- Updated generative process

  (1) Draw coefficients $\beta \sim \mathcal{N}(\beta|\mathbf{0}, \lambda\mathbf{I})$
  (2) For each feature vector $\mathbf{x}_n$

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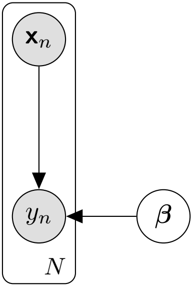

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- Joint probability distribution becomes

$$p(\mathbf{y}, \beta|\mathbf{X}, \lambda) = p(\boldsymbol{\beta}|\lambda) \prod_{n=1}^{N} p(y_n|\boldsymbol{\beta}, \mathbf{x}_n)$$

$$= \underbrace{\mathcal{N}(\boldsymbol{\beta}|\mathbf{0}, \lambda\mathbf{I})}_{\text{prior}} \times \underbrace{\prod_{n=1}^{N} \text{Poisson}(y_n|e^{\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n})}_{\text{likelihood}}$$

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- Exact inference is no longer tractable
- Must resort to **approximate inference** methods
- Not a problem for Stan :-)

Playtime!

- Poisson regression model of taxi pickups in NYC
- See “05 - Regression models - Part 2.ipynb" notebook
- Do part 2.2
- Expected duration: 30 minutes

Going back to the modelling assumptions...

- Suppose that Gaussian was indeed the most appropriate distribution for the target variable y

$$y_n \sim \mathcal{N}(y_n | \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_n, \sigma^2)$$

- What if our observations of y had **non-constant noise**?

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- Suppose that Gaussian was indeed the most appropriate distribution for the target variable y

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- What if our observations of y had **non-constant noise**?
- Consider the problem of modelling traffic speed data from probe vehicles
- The assumption of constant observation noise σ^2 might be too strong!

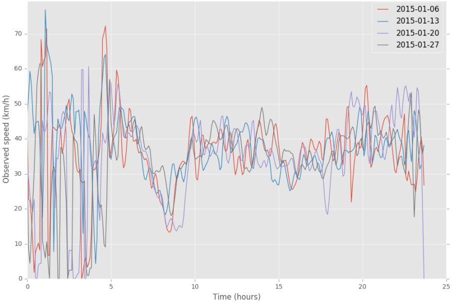

Figure: Traffic speeds in a road segment in Nørreport

Heteroscedastic regression

- We can relax the constant observation noise assumption by making the variance (linearly) dependent on a set of arbitrary features $\mathbf{z}$ (e.g. time of the day)

$$y_n \sim \mathcal{N}(y_n | \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_n, e^{\boldsymbol{\eta}^\mathsf{T} \mathbf{z}_n})$$

  where $\boldsymbol{\eta}$ is a new set of coefficients to parameterize the relation between the features $\mathbf{z}$ and the observation noise

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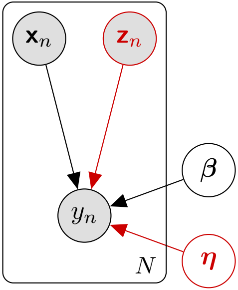
- As with the Poisson, we use a log link function to ensure non-negative variances

$$e^{\boldsymbol{\eta}^\mathsf{T}\mathbf{z}_n} \in (0, \infty)$$

- This allows to account for things like **time-varying observation noise** and produce better **uncertainty estimates** for the predictions!
    - Useful to know how reliable the predictions are

Bayesian heteroscedastic regression model

- Updated graphical model



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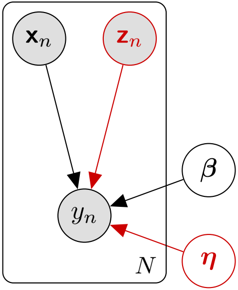

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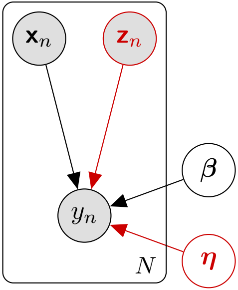

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Beyond linearity...

- So far we have been assuming a linear relationship between y_n and $\mathbf{x}_n$, such that

$$y_n \sim f(\mathbf{x}_n) + \epsilon$$

  where $f(\mathbf{x}_n) = \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_n$

- As previously explained this is far more powerful than it looks at first sight!
- However, in some cases, it might still not be enough... But what can we do?

[1] https://arxiv.org/abs/1411.2581

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- However, in some cases, it might still not be enough... But what can we do?
- We can assume $f(\mathbf{x}_n)$ to be a complex **deep neural network**!
  - In fact, we can parametrize any exponential family distribution using a DNN
    - Check out, e.g.: *Deep Exponential Families*[1]
  - Intersection between Deep Learning and Bayesian methods is currently a very popular research topic!
  - Out the scope of this course (unfortunately!)
  - Beyond STAN's current capabilities

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[2] http://www.gaussianprocess.org/gpml/

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  where $f(\mathbf{x}_n) = \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_n$
- **Gaussian processes** (GPs) allow us to model **non-linear** relationships!
  - **Non-parametric** models
  - Provide a probability distribution over functions
  - Place Gaussian process prior on the function f: $f \sim \mathcal{GP}$
  - GP prior specifies characteristics of the function, like stationarity, smoothness, periodicity, etc.
  - Unfortunately, no time to cover them in detail (as they deserve!)
  - "Gaussian Processes for Machine Learning" book is a great resource![2]
  - Also, check out the STAN manual if you're interested

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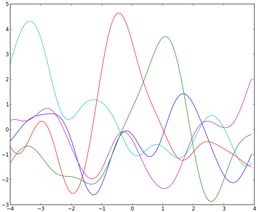
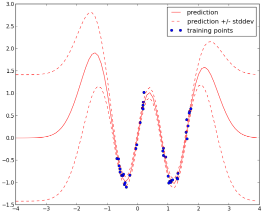
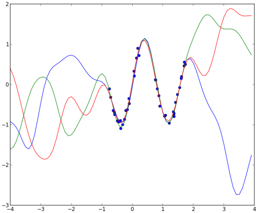
Beyond linearity...



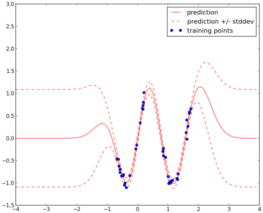
(a) samples from the GP prior



(b) predictive posterior



(c) samples from the GP posterior



(d) pred. post. after hyper-param. optimization

Playtime!

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