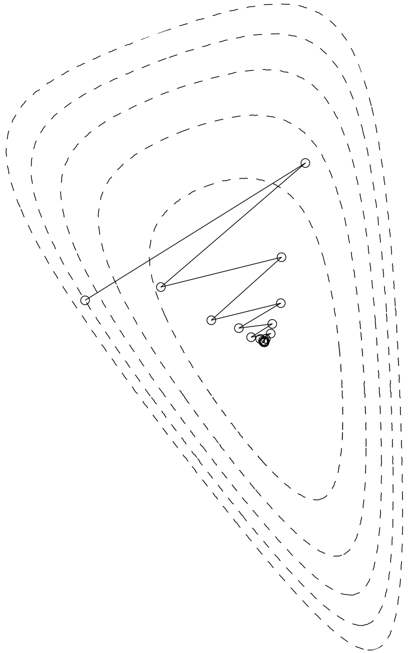

Optimization Algorithms

No Free Lunch

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Winter 2024/25

References

- Toussaint: *The Bayesian Search Game*. In Theory and Principled Methods for Designing Metaheuristics, Springer, 2012.
- Igel & Toussaint: *On Classes of Functions for which No Free Lunch Results Hold*. Information Processing Letters, 86, p. 317-321, 2003.
- Wolpert & Macready. *No free lunch theorems for optimization*. IEEE Transactions on Evolutionary Computation, 1(1):67–82, 1997.

No Free Lunch Theorem – Problem Setting

[Following *The Bayesian Search Game* (2012)]

- Finite(!) space X
- Distribution $P(f)$ over functions $f:\ X \to Y$
- A **non-revisiting** algorithm $\mathcal{A}$ generates queries x_t and observations $y_t = f(x_t)$. Formally, a probabilistic algorithm is defined by

$$P(x_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A})$$

  and $P(x_1; \mathcal{A})$.

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  and $P(x_1; \mathcal{A})$.
- Therefore, $\mathcal{A}$ interacting with random function f generates the joint process:

$$P(f, x_{1:T}, y_{1:T}; \mathcal{A}) = P(f)\ P(y_1 \,|\, x_1, f)\ P(x_1; \mathcal{A})\ \prod_{t=2}^{T} P(y_t \,|\, x_t, f)\ P(x_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A})$$

No Free Lunch Theorem

- **Theorem:**

$$\exists h : Y \to \mathbb{R} \text{ s.t. } \forall K \in \mathcal{N}^+, \{x_1, .., x_K\} \subset X :\ P(f_{x_1}, .., f_{x_K}) = \prod_{k=1}^{K} h(f_{x_k}) \qquad (1)$$

$$\iff \qquad \forall_{\mathcal{A}}, \forall_T :\ P(y_{1:T}; \mathcal{A}) = \prod_{i=1}^{T} h(y_i) \quad \text{(independent of } \mathcal{A}\text{)} \qquad (2)$$

- In words:
  $P(f)$ factorizes $\quad \Leftrightarrow \quad$ all $\mathcal{A}$ generate the same random observations

[Proof later]

No Free Lunch Theorem – Comments

- Interpreting the LHS:
  - $P(f_{x_1},..,f_{x_K}) = \prod_{k=1}^K h(f_{x_k})$ factorizes i.i.d.
  - **There is no mutual information between any** $f(x_1), f(x_2), x_1 \neq x_2$, $I(f(x_1), f(x_2)) = 0$
  - Observing $f(x_1)$ reveals no information whatsoever on what $f(x_2)$ might be
  - Any (non-repeating!) algorithm is equally blind and uninformed about what future observations might be, not matter how it collected past information $(x_{1:t\text{-}1}, y_{1:t\text{-}1})$

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- Often we have a performance metric (see later); but "all observations $P(y_t \mid ...; \mathcal{A})$ are indep. of $\mathcal{A}$" is stronger and implies equal expected performance with whatever metric
- Traditional statement: "Averaged over *all* problem instances, any algorithm performs equally. (E.g. equal to random.)"
- "there is no one algorithm that works best for every problem"

No Free Lunch Theorem – Comments

- The classical citation is Wolpert & Macready (1997), but is less general than the above and proof overly complicated and less clear in my view.
  - "Averaging over all problems" $\rightarrow$ expectation w.r.t. $P(f)$
  - "set of functions closed under permutation" $\rightarrow$ $P(f)$ factorizes
  - Our Theorem is strong $\Leftrightarrow$, not just $\Rightarrow$ (Igel & Toussaint, 2004)

NFL Proof

- We defined the process $P(f, x_{1:T}, y_{1:T}; \mathcal{A})$ previously
- Basic definitions of probabilities to prove $\Rightarrow$:

$$\begin{aligned}
P(y_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A}) &= \sum_{x_t \in X} \Big[\sum_f P(y_t \,|\, x_t, f)\ P(f \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}) \Big]\ P(x_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A}) \\
&= \sum_{x_t \in X} P(f_{x_t} \!=\! y_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1})\ P(x_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A}) \\
&= \sum_{x_t \in X} h(y_t)\ P(x_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A}) = h(y_t)\ .
\end{aligned}$$

Last line: $\mathcal{A}$ is non-revisiting, and $P(f_{x_t} \!=\! y_t \,|\, x_{1:t\text{-}1}, y_{1:t\text{-}1}) = P(f_{x_t} \!=\! y_t) = h(y_t)$.

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\end{aligned}
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- Prove $\Leftarrow$ by explicitly constructing algorithms that generate different outputs when $P(f)$ is non-factored. [Details in *The Bayesian Search Game*, 2012]

No Free Lunch for Optimization

- Consider the problem $\min_{x \in X} f(x)$ for finite X
- Also here, an algorithm $\mathcal{A}$ is defined by $P(x_k \mid x_{1:t\text{-}1}, y_{1:t\text{-}1}; \mathcal{A})$
- A typical performance metric could be **regret**

$$R(T) = \sum_{t=1}^{T} y_t - y^*$$

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- A typical performance metric could be **regret**

$$R(T) = \sum_{t=1}^{T} y_t - y^*$$

- But if for a non-repeating(!) $\mathcal{A}$, $P(y_t)$ is indep. of $\mathcal{A}$, so is the expected regret

No Free Lunch for Machine Learning

- Given data $D = \{(x_i, y_i)\}_{i=1}^n$, find a predictor $\hat f : \ X \to y$ that minimizes expected loss $\mathbb{E}\Big\{\ell(\hat f(x^*), f(x^*))\Big\}$ for a future query x^*, where $f(x^*)$ is the ground truth
- A learning algorithm $\mathcal{A}$ is a predictive distribution $P(y \,|\, x^*, D; \mathcal{A})$ (i.e., a mapping from D to a prediction $P(y \,|\, x^*)$ for a new query x^*)
- Assume X is finite and $x^* \notin D$ (non-repeating!)

- But if $P(f)$ factorizes so that $P(f(x^*){=}y) = h(y)$ is fully independent from D (zero mutual information), then no algorithm can learn anything or predict better than the prior.

Bayes' Theorem

$$P(X|D) = \frac{P(D|X)}{P(D)}\, P(X)$$

$$\text{posterior} = \frac{\text{likelihood} \cdot \text{prior}}{\text{normalization}}$$

- But if X is indep. from D, then there is nothing to learn or predict better than the prior $P(X)$

Conclusions from NFL?

- NFL is an almost trivial theorem, what is non-trivial is what to make of it

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- First pressing question:
  - Does NFL also hold for continuous X? What would it mean that $P(f)$ is factorized, or $I(f(x_1), f(x_2)) = 0$, for any $x_1 \neq x_2$ in continous X?

- NFL is an almost trivial theorem, what is non-trivial is what to make of it

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- Thoughts on conclusions from NFL:
  - Become aware, in your methods, what actually you are assuming - you must assume something
  - Fight back if anybody ever states "we don't (want to) make assumptions" (e.g. in a talk on RL that claims it can solve any problem without assumptions)
  - There is no Artificial General Intelligence if general would mean "making NO assumptions". So, the AGI community (say, Marcus Hutter) must make some assumptions – what are they *exactly*?
  - What are assumptions we would "generally" accept to make in our physical universe? (In case we care about AI specifically in our physical universe.)
  - What are algorithms that literally start by making assumptions about $P(f)$ and then derive an optimal algorithm for that $P(f)$? (see Bayesian Search Game...)

NFL in continuous domains

- The LHS describes $P(f)$ with $I(f(x_1), f(x_2)) = 0$ for any $x_1 \neq x_2$
  - How can we define probability distributions over functions (over continuous X) in the first place?

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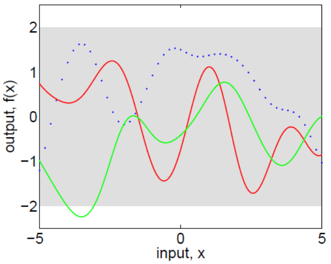
  - How can we define probability distributions over functions (over continuous X) in the first place?

- A typical way to define distributions over $f : \mathbb{R}^n \to \mathbb{R}$ is as a **Gaussian Process**:
  - For every finite set $\{x_1, .., x_M\}$, the function values $f(x_1), .., f(x_M)$ are Gaussian distributed with mean and covariance

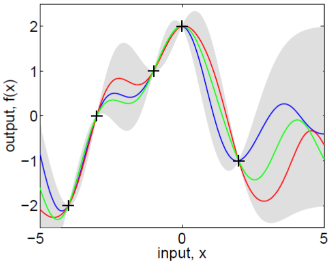
$$\mathbb{E}\{f(x_i)\} = \mu(x_i) \qquad \text{(often zero)}$$
$$\mathbb{E}\{[f(x_i) - \mu(x_i)][f(x_j) - \mu(x_j)]\} = k(x_i, x_j)$$

    where, $\mu(x)$ is called **mean function**, and $k(x, x')$ is called **covariance function**
  - μ and k generalize the notion of *mean vector* μ_x and *covariance matrix* $\Sigma_{xx'}$ from finite $x \in \{1, .., n\}$ to continuous $x \in \mathbb{R}^n$

GP examples



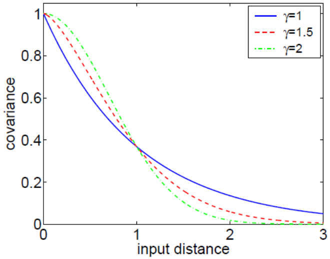
(a), prior

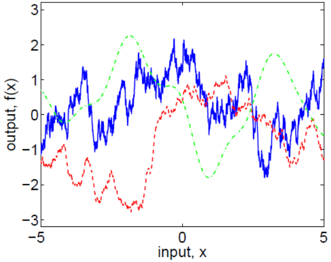


(b), posterior

(from Rasmussen & Williams)

GP examples: different covariance functions





(from Rasmussen & Williams)

- These are examples from the γ-exponential covariance function

$$k(x, x') = \exp\{-|(x - x')/l|^\gamma\}$$

NFL in continuous domains

- Back to NFL: the LHS requires $I(f(x_1), f(x_2)) = 0$, which would mean, for GPs, zero covariance function $k(x, x') = 0$ for any $x \neq x'$

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- At first sight this might seem ok, but
  - Auger & Teytaud clarify that "zero-covariance GP" is not a proper Lebesgue measure over function
  - Conversely, they state that for any Lebesgue meassure the LHS does not hold (and claim that Lebesgue meassures are the only sensible kind of $P(f)$)

A. Auger and O. Teytaud: *Continuous lunches are free plus the design of optimal optimization algorithms.* Algorithmica, 2008

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- Beyond my expertise as non-mathematician
- But the point of NFL remains the same: one would only have to replace "non-revisiting" by "non-near-revisiting" or so.

NFL in continuous domains – conclusions

- Whether NFL holds in continuous domains depends on what $P(f)$ you consider mathematically sound
- The core point remains that if $I(f(x_1), f(x_2)) = 0$ (for non-close x_1, x_2), no non-(near)-revisiting algorithm can be smart

- Gaussian Processes are the simplest instance for assuming non-zero $I(f(x_1), f(x_2)) \neq 0$, by assuming Gaussian dependencies between $x \neq x'$
  $\Rightarrow$ GPs became a standard assumption to explicitly design algorithms exploiting that assumption and evading NFL

Become aware, in your methods, what actually you are assuming - you must assume something

- What did our optimization algorithms assume so far?

Assumptions in continuous optimization

- f is continously differentiable $f \in C^1$!
  - The limits exist! Clearly there are "correlations" when approaching infinitesimally!
  - Sure we can predict to (infinitesimally close) points: The gradient gives an accurate 1st order Taylor prediction (in the vicinity)
  - We can predict to go downhill following the gradient.
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- All assumptions are *local*, and were used to characterize local convergence behavior

Assumptions made in AGI

- Kolmogorov & Solomonoff complexity
  (also not my expertise...)

  Lattimore & Hutter: *No free lunch versus Occam's razor in supervised learning*. In Algorithmic Probability and Friends. Bayesian Prediction and Artificial Intelligence, 2013

  Baum, Hutter, & Kitzelmann: *Artificial general intelligence*. In Proceedings of the Third Conference on Artificial General Intelligence, 2010

- Occam's rasor: $P(f)$ is higher for "simpler" functions f. Assuming all (relevant) f are computable, simpler = of lower Kolmogorov/Solomonoff complexity.
- Obvious algorithm to exploit this universal prior: Sort all f by complexity, test each in order – will be better than random.
- Can also define optimal algorithms (optimal AGI) under this universal complexity prior

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  - physics $\leftrightarrow$ space$\times$time; things (fields/objects); local(!) interactions between things; invariances(!)
  - images $\leftrightarrow$ invariances; neighboring pixels correlated $\leftrightarrow$ convolutional features, hierarchies, CNN
  - time series $\leftrightarrow$ Markovian, maybe smooth $\leftrightarrow$ HMMs, MDPs, control, etc, etc
  - Robotics, Language, Text, humans, animals, etc etc

What are algorithms that literally start by making assumptions about $P(f)$ and then derive an optimal algorithm for that $P(f)$?

Optimal Optimization

- Optimization can be formalized as a sequential decision problem (MDP):
  - Start with a prior $b_0 = P(f)$
  - Choose a query x_t based on b_t (policy, acquisition function)
  - Query x_t, observe y_t, update data D, update belief $b_t \leftarrow P(f \mid D)$, iterate

$$\begin{tikzcd}
b_0 \arrow[rr] \arrow[dr] & & b_1 \arrow[rr] \arrow[dr] & & b_2 & \cdots \arrow[dr, dashed] & & \\
& x_1 \arrow[ur] \arrow[r] & y_1 \arrow[u] & x_2 \arrow[ur] \arrow[r] & y_2 \arrow[u] & \cdots & x_T \arrow[dr] & \\
f \arrow[rrrrrrr] \arrow[uurr, bend right] \arrow[uurrrr, bend right] & & & & & & & R
\end{tikzcd}$$

[Bayesian Search Game]

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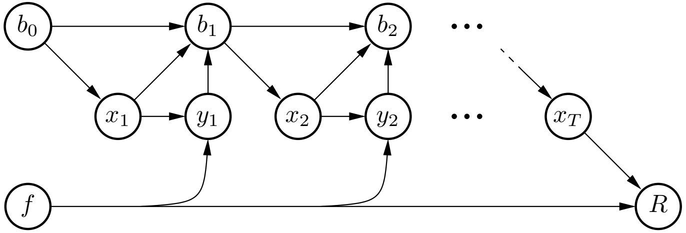

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f \arrow[urr] \arrow[urrrr] \arrow[rrrrrr] & & & & & & R
\end{tikzcd}$$

[Bayesian Search Game]

- This defines a *known* decision process, for which we can define an optimal policy
  - Can in principle be computed using Dynamic Programming – but intractable

Bayesian Optimization in a nutshell

- We maintain a particular belief $b_t = P(f \mid D)$, namely a *Gaussian Process*

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- We maintain a particular belief $b_t = P(f \mid D)$, namely a *Gaussian Process*

- Don't plan an optimal query policy, but use a 1-step heuristic:
- An **acquisition function** $\alpha(x, b_t)$ characterizes how "interesting" it is to query x next, and defines the policy

$$x_t = \operatorname*{argmax}_x \alpha(x, b_t)$$

- Analogies:
  - $\alpha(x, b_t)$ is a descriminative function for the next decision
  - $\alpha(x, b_t)$ is like a Q-function $Q(b_t, x)$ for the next decision (but not learned)

to be continued with Bayesian Optimization...