Wasserstein Consensus for Bayesian Sample Size Determination

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Sample Size Determination

the big picture

Pre-sperimental problem consisting of **choosing the size of the sample,** n, typically trying to minimize uncertainty under some cost constraint.

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GOAL: find a sample size that induces agreement between different parties

The (bayesian) state of the art

the main ingredients

- Analysis Prior $\pi_A(\theta)$:

  models pre-experimental information to be used to obtain the **posterior distribution**

- Design Prior $\pi_D(\theta)$:

  models uncertainty on the experiment to be used to obtain the **predictive distribution**

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Select n in order to satisfy some inferential goal, to be formalized in terms of a summary of the posteriors

$$\rho_{\pi_A}(\theta|y_n) = \int g(\theta)\pi_A(\theta|y_n)\mathrm{d}\theta$$

The (bayesian) state of the art

in the two prior approach

The design predictive distribution $m_D(y)$ removes the dependency of $\rho_{\pi_A}(\theta|y_n)$ from the observed sample y_n

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- **PEC** - Predictive Expectation Criterion

$$e(n) = \mathbb{E}_{m_D}[\rho_{\pi_A}(\theta|Y_n)] \qquad n^* = \min\{n \in \mathbb{N} : e(n) > \eta\}$$

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η and γ are clinically relevant thresholds and depend on the problem.

Multiple priors

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- diverging expert opinions
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Community of priors problem: how to combine multiple sources of pre-sperimental information into the analysis?

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mixtures of priors

Aggregate multiple priors into one and then use the approach of your likings.

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$$\pi_A(\theta|y_n) = \sum_{i=1}^{K} \frac{\omega_{0,i} m_i(y_n)}{\sum_{r=1}^{K} \omega_{0,r} m_r(y_n)} \times \pi_i(\theta|y_n)$$

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Will the *i*-th clinician believe us?

Brutti, P., De Santis, F., & Gubbiotti, S. (2009). *Mixtures of prior distributions for predictive Bayesian sample size calculations in clinical trials.* Statistics in medicine

Our Solution

enforcing “consensus” between sources

- (possibly) conflicting priors π_1, π_2
- resulting posteriors $\pi_{1,y}, \pi_{2,y}$

Two experts “agree” if their inferential conclusions are the same

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We formalize **agreement** or **consensus** in terms of distance between $\pi_{1,y}$ and $\pi_{2,y}$

Formally

how does this relate to the standard framework?

We can still adopt the Predictive approach, as this it's just another way of defining the summary statistic:

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we just need to pick a distance

Wasserstein distance

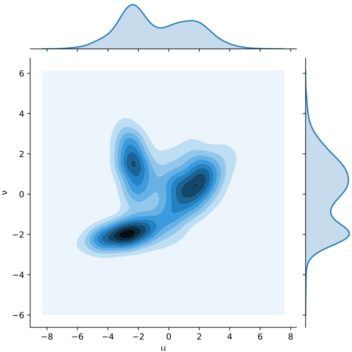
a.k.a. Kantorovic, Earth Mover

$(p, d)-$ **Wasserstein distance**

$X \sim P$ and $Y \sim Q$, $p \geqslant 1$ and d ground distance

$$W_{d,p}(P, Q) = \left(\inf_J \int_{\mathcal{X} \times \mathcal{Y}} d(x, y)^p \; \mathrm{d}J(x, y) \right)^{1/p}$$

where the infimum is over **all joint** distributions J having P and Q as marginals.



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it's this popular for a good reason

- it "metricises" convergence in distribution

    if two distributions are close w.r.t. the Wasserstein distance they are probabilistically similar.

Verdinelli, I., Wasserman, L. (2018) Hybrid Wasserstein Distance and Fast Distribution Clustering. *arXiv preprint arXiv:1812.11026*

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- it is sensible to the geometry of the space

  it's not just about the location!

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Multivariate Gaussian distributions

computing the Wasserstein distance

Let $X \sim \mathrm{N}(\boldsymbol{\mu}_X, \boldsymbol{\Sigma}_X)$ and $Y \sim \mathrm{N}(\boldsymbol{\mu}_Y, \boldsymbol{\Sigma}_Y)$, when **the ground distance is taken to be the L_2 distance**, we have a closed form expression for Wasserstein:

$$\mathrm{W}_{L^2,2}(X, Y) = \|\boldsymbol{\mu}_X - \boldsymbol{\mu}_Y\|_2^2 + \mathtt{B}^2(\boldsymbol{\Sigma}_X, \boldsymbol{\Sigma}_Y)$$

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distance between the means **+** distance between the variances

Conjugate Univariate Gaussian Model

computing the Wasserstein distance

Likelihood: $\mathsf{N}(\theta, \sigma^2)$, with σ^2 known.

$$\pi(\theta) = \mathsf{N}\left(\theta; \mu_0, \frac{\sigma^2}{n_0}\right)$$

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If we have two priors, Wasserstein between the corresponding posteriors is:

$$\mathrm{W}_{L^2,2}(\pi_{1,y}, \pi_{2,y}) = (\mu_{1,\mathrm{P}} - \mu_{2,\mathrm{P}})^2 + (\sigma_{1,\mathrm{P}} - \sigma_{2,\mathrm{P}})^2 .$$

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in the Bayesian predictive approach to SSD

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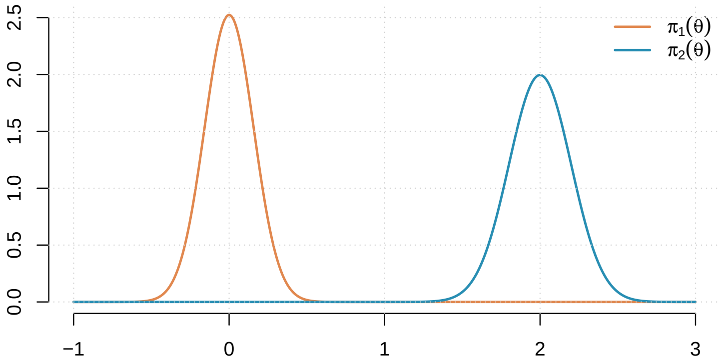
PPC: $$p_{1,2}(n) = 1 - F_{\chi^2} \left(\frac{\gamma - \mathrm{B}^2_{\sigma^2}}{\widetilde{\sigma}^2}; df = 1, \widetilde{\mu}^2 \right)$$

- $w_1 = n_1/(n+n_1)$
- $w_2 = n_2/(n+n_2)$
- $w_n = (1-w_1) - (1-w_2)$
- $\widetilde{\mu} = w_1\mu_1 - w_2\mu_2 + w_n\mu_D$
- $\widetilde{\sigma}^2 = w_n^2\sigma^2(1/n + 1/n_{\mathrm{D}})$
- $\mathrm{B}^2_{\sigma^2} = (\sigma_{1,\mathrm{P}} - \sigma_{1,\mathrm{P}})^2$

A Toy Example

mildly informative priors

$$\pi_1(\theta) = \mathrm{N}(0, 2/80) \qquad \pi_2(\theta) = \mathrm{N}(2, 2/50)$$



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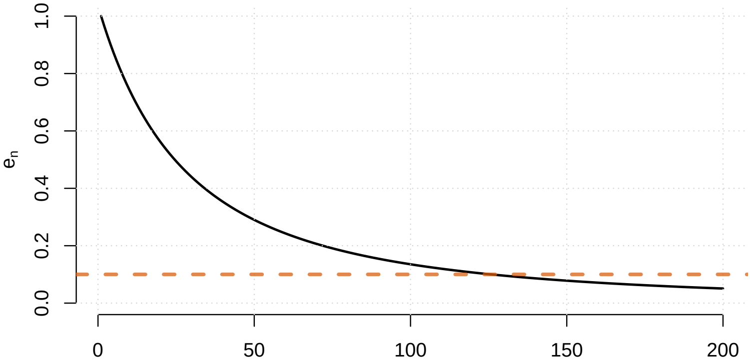
$\eta = 0.1$ $\quad$ $n^* = 125$



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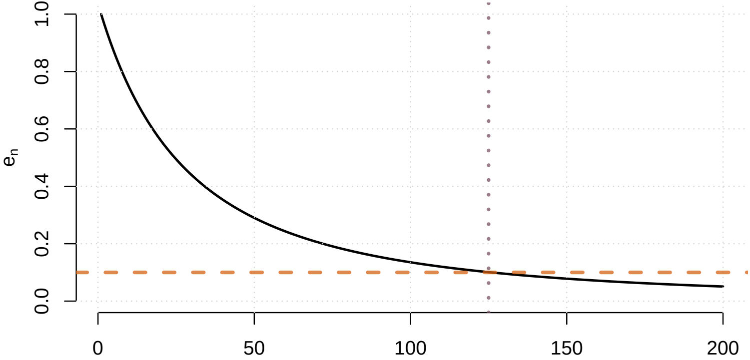
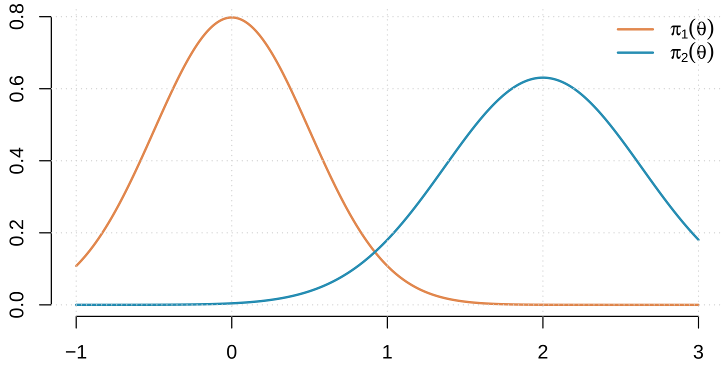


Another Toy Example

weakly informative priors

$$\pi_1(\theta) = \mathrm{N}(0, 2/8) \qquad \pi_2(\theta) = \mathrm{N}(2, 2/5)$$



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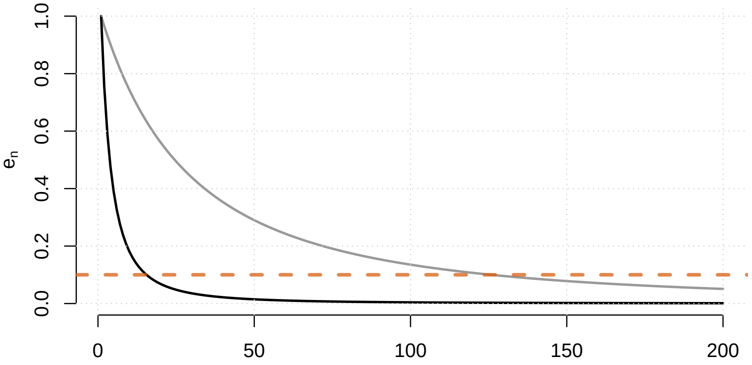
$\eta = 0.1$ $n^* = 15$



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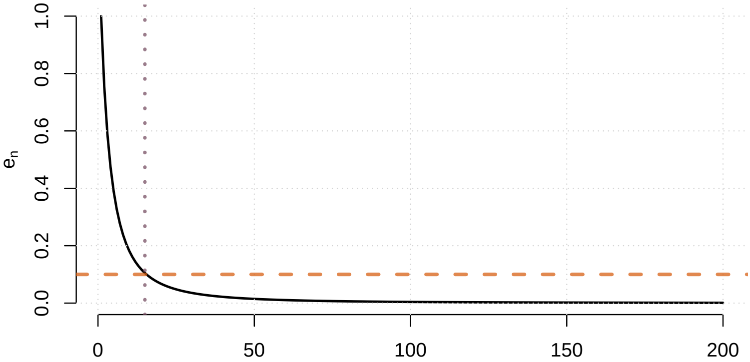

How to select η?

a small bump in the road

Given a $\beta \in (0, 1)$, choose η as

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When this happens

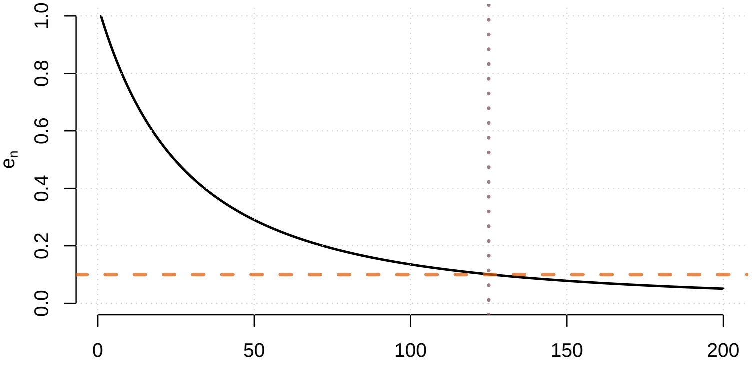
$$\arg\max_n e_{1,2}(n) = e_{1,2}(1)$$

β represent how much difference we can tolerate with respect to the minimum sample size possible.

A Toy Example

Reprise

$\eta = 0.1$ $n^* = 125$



A Real Data Example

from Spiegelhlter et al. (2004)

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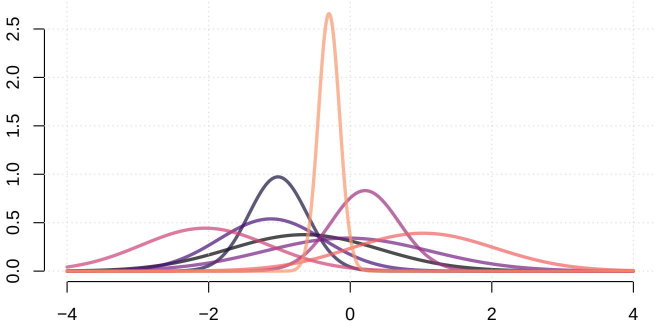
A bunch of priors encoding evidence from previous experiments:



An Unfair Comparison

was this really necessary?

- **Likelihood** Gaussian with unknown mean θ and $\sigma^2 = 4$
- **Design Prior** Gaussian with mean $\mu_D = 0.058$ and variance σ^2/n_D
- **Threshold** $\eta = 0.05$

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$\boldsymbol{n_D}$	$\boldsymbol{n^*_{\texttt{WASS}}}$
4319	361
432	371
43	468

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n_D	$n^*_{\texttt{WASS}}$	$n^*_{\texttt{MIXT}}$
4319	361	498
432	371	509
43	468	190

Consensus does not typically come "for free"

Brutti, P., De Santis, F., & Gubbiotti, S. (2009). *Mixtures of prior distributions for predictive Bayesian sample size calculations in clinical trials.* Statistics in medicine

Conjugate Beta-Binomial

moving beyond gaussianity

When the posterior distributions are not Gaussian, the Wasserstein distance does not necessarily have an analyitic expression.

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Possible solutions are:

- Numerical evaluation of the Wasserstein distance
- Approximation of the Wasserstein distance via Stein's method

Stein’s method

quickest introduction ever

X, Y random variables (typically X is "what you have", Y is "what you want")

1. rewrite the distance between X and Y as the **expectation** of a functional $h(X)$

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If we compare X and Y via the L_1 Wasserstein distance, we can derive tight bounds for it.

Ley, C., Reinert, G., & Swan, Y. (2017). Stein's method for comparison of univariate distributions. *Probability Surveys*.

Stein's bound for the B-B case

the second most famous framework in clinical trials

Likelihood: Binomial(θ, N), T events in the sample.

$$\pi(\theta) = \text{Beta}\,(\theta; \alpha, \beta)$$

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$$d_W(\pi_{1,y}, \pi_{2,y}) \leq \frac{|\alpha_1 - \alpha_2|}{\alpha_1 + \beta_1 + n}(1 - \mu_{2,P}) + \frac{|\beta_2 - \beta_1|}{\alpha_1 + \beta_1 + n}\mu_{2,P}$$

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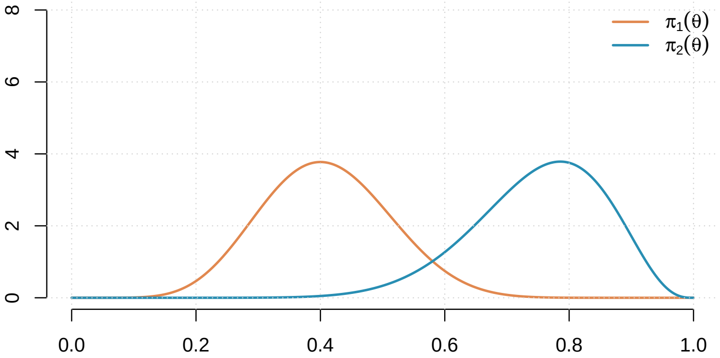
If we assume $\pi_D(\theta) = \text{Beta}(\theta; \alpha_D, \beta_D)$ it is possible to bound the **PEC** and **PPC** just by remembering:

$$\mathbb{E}_{m_D}[T] = \frac{n\alpha_D}{\alpha_D + \beta_D}$$

Yet Another Toy Example

the more the merrier

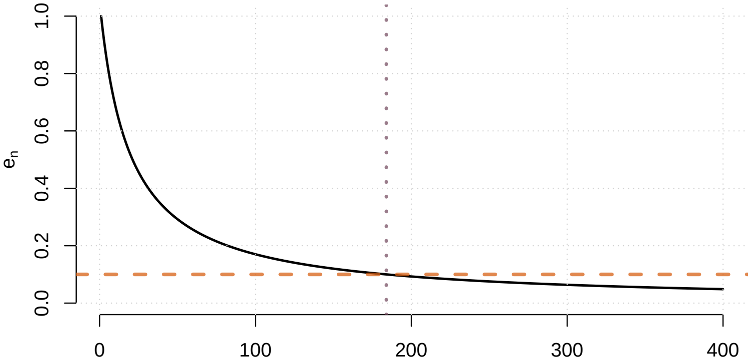
$$\pi_1(\theta) = \text{Beta}(9, 13) \qquad \pi_2(\theta) = \text{Beta}(12, 4)$$



Yet Another Toy Example

the more the merrier

$\eta = 0.1$ $\quad\quad$ $n^* = 184$



R-package coming soon!

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Thanks!

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